Simulation chain of material simulation, heat treatment simulation and welding simulation for industrial application

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1 Introduction

Heat is used for welding and during heat treatment. In both processes the material properties change due to temperature gradients and resulting microstructure change. A physically realistic simulation has to consider the interaction of process model and material model.

The simulation chain material - heat treatment - welding enables the prediction of the state and the characteristics of products. Additionally, it can also enable the design of products from scratch - without any physical test. Design parameters would be the chemical composition of the alloy as well as the process parameters for welding and heat treatment.

Material properties depend on microstructural evolution which results from both chemical composition and process history. The evolution of the microstructure during processing depends on a chain of T/t cycles with different heating and cooling rates. Resulting thermo-physical and mechanical properties can be calculated using JMatPro® [1]. State-of-the-art ICME (Integrated Computational Materials Engineering) tools like Matplus EDA® can bring together data from materials testing, materials simulation and materials reference databases. Hybrid material models can be created, which use information from testing, constitutive equations and materials simulation [2]. By that EDA® can be used as a system which provides different specific material cards for welding and heat treatment simulation.

The practical use of the targeted complex simulations in industrial environments requires user-friendly pre- and post-processors. Using state-of-the-art materials information and FEA-solvers as a starting point the authors developed solutions for different applications which facilitate the simulation of complex processes so that they can also be used by non finite element experts.

MatPlusHQ links material simulation and the thermal part of heat treatment simulation. It is an easy-to-use tool for industrial shop floor which helps users to predict heating and quenching of complex parts in order to increase productivity and reduce energy consumption.

DynaWeld® is a more complex preprocessor for high sophisticated simulations of the entire process chain. Addressing the LS-DYNA® code DynaWeld® simulation models connect the thermal solution, mechanical distortion, residual stress, strain hardening or stress release, material phase proportion and hardness.

2 MatPlusHQ - Heating and Quenching simulations

A challenge in industrial practice is the optimum heating rate of components in furnaces during heat treatment: When is a homogeneous target temperature reached and which thermal stresses result from temperature differences during heating?

Small batches and individual parts usually do not allow any experimental optimization of the heating cycle.

Without simulation users tend to be on the safe side and take slower heating rates and longer holding times than physically required. This results in unnecessary costs of energy and decreased productivity. Benchmarks in foundries have shown significant saving potentials of more than 25%.
These savings can also result in reduced capital costs – buying of new furnaces may be not necessary if productivity of existing equipment can be increased.

From a scientific point of view, this optimization task is a simple one – taking into account all the state-of-the-art FEM (Finite Element Method) simulation systems. Many powerful programs can handle this optimization task. But software-costs as well as costs and availability of appropriate scientific personnel usually prevent their use in industrial practice.

For this reason, an innovative simulation program has been developed which takes into account the requirements of practical users on the shop floor [3]:

- Easy operation also for machine operators
- Fast results in minutes on standard PC's
- Suitability for practice-relevant geometries and materials data

MatPlusHQ thus enables optimization of energy consumption and productivity through sophisticated simulation on workshop level:

Machine operators can improve process schedules based on information from simulation in line with their operational experience.

**Fig.1: Basic geometries in MatplusHQ and autogenerated mesh**

Thus, the above-mentioned potentials can be achieved by the optimal temperature-time course. This applies both to existing furnaces as well as for new investments. MatPlusHQ runs complex 3-D FEM calculation automatically in the background. Based on 3-D geometries, which can be imported from CAD systems using IGES/STEP, an automatic and fast meshing is performed – the mesh is optimized for computational speed. Optionally, the user can also visually inspect and influence the quality of the mesh. For simple cases, the use of basic shapes, such as sphere, cylinder or cuboid is possible.
Figure 1 shows an example of some basic geometries and a 3-D mesh based on the geometry of a pilgrim roller. For the different applications of heating and cooling, the system provides preconfigured and temperature-dependent heat transfer coefficients. With the appropriate authorization, these data can also be adapted by the user to the current boundary conditions of the existing system technology.

The temperature-dependent materials data (density, heat capacity and thermal conductivity) play an important role in the calculation. These data can be calculated using the JMatPro® software [4] and imported to the system.

A direct integration of the calculation of material data using the JMatPro® API is also implemented: In this way the influences of analysis deviations on the heat treatment can be calculated with exact data [5]. The current version takes into account the phase transformation in steels - however, the integration of data from TTT diagrams is planned for a later version.

Figure 2: User interface with results

Figure 2 shows the user interface of the software after a heating simulation. Strong emphasis was placed on a clear user interface, so that an operation can also be done via touchpad or tablet computer. Informative graphics show the heating of the coldest point in the component in relation to the furnace chamber and component surface as well as the resulting temperature differences over the process time.

High temperature gradients on the component surface are to be expected in cooling down simulations, in particular if quenching media with high heat transfer coefficients, such as water or oil are used. In this case, an automated grid generation optimized for computation time is often insufficient.

Because of this reason meshes with a boundary-layer structure can be imported, so that such calculations can be carried out successfully. Given the fact that during cooling processes the material properties depend to a large extent on the cooling rate that occurs, an iterative process is used to determine the cooling rate. In Figure 3 the dependence of the cooling rate on the materials properties (here: density of AISI 3310) is illustrated. In a first step, the simulation is carried out with materials properties in thermal equilibrium. From the resulting cooling time an average cooling rate is calculated and used to generate new materials data records for the following simulation. This iterative process usually converges after only two iterations.
3 Material data preparation with DynaWeld®

The material simulation provides the material properties against temperature for the basic microstructural components which are handled like phases. In case of steel the microstructures are: austenite, ferrite, perlite, bainite and martensite. The initial state of the material can be considered as a mixture of these phases. The material properties are calculated using the properties of the phases and applying appropriate mixture rules. For the simulation of welding processes with filler material a special phase is needed to consider the not yet deposit material. The main property of this material is to have no stiffness, which is approached with a low young modulus. Another phase indicates molten material.

Tempered phases can be added by DynaWeld®-Material if they are not part of the source data. Softening by annealing can be included by decreasing the flow curves (yield and tensile stress) of the individual phases. JMatPro® allows the calculation of tempering of martensite which can be used to adjust the flow stress curves. Annealing or tempering of bainite is complex and does usually not happen in welding processes due to short times.

Figure 4 explains the work flow for material import, adjustment and preparation. The raw data comes from materials simulation. The information of material specification is used to adjust the base material. For simulation reasons some special settings for the materials data must be considered in order to provide a robust simulation run. With the melting of material, the strain hardening is erased and requires a definition in the FEM material model. These are welding and heat treatment specific parameter as additional input to the basic material data.

Special criterions like crack risk or damage indication and the formula for hardening calculation expand the data set. The management of the FEM-internal material dataset ID is required to manage multi materials in one simulation model. Initial strain hardening coming for example by prior milling process is considered by setting initial plastic strain.

The DynaWeld® material tool collects the additional data and settings, expands the basic phases by base material, liquid phase and tempered phases and generates the material card for welding and heat treatment FEM analysis:

- the LS-DYNA multiphase material model *MAT_GENERAL_PHASE_CHANGE (*MAT_254) [6]
- the LS-DYNA single material model *MAT_CWM (*MAT_270)
The single material model is applicable for welding distortion analysis. The multi-phase is reduced to a single phase with special approach for phase transformation strain.

Fig. 4: Flowchart material preparation of DynaWeld®

Fig. 5: Flow curve adjustment considering yield and tensile stress

An adjustment algorithm used is based on an approach by Loose [7] which is explained in figure 5. This approach postulates that the ratio of yield and tensile stress between two phases at room temperature is the same as at higher temperature. A given flow curve (basic curve) is transformed to the adjusted curve by yield stress and tensile stress. The flow curve is therefore divided in two parts: elastic and plastic. Both parts are adjusted separately. The elastic part is adjusted by the ratio of yield stress. The plastic part is adjusted by the ratio of strain hardening, which is the difference between tensile stress and yield stress. Finally, the adjusted parts are joined to a new flow curve.

JMatPro® uses the Kirkaldy model for the predictive calculation of phase transformation. For the FEM analysis a descriptive model provides the advantage to describe arbitrary given transformations. This method is applicable also on drawn CCT-Diagrams. The generalized Johnson-Mehl-Avrami-
Kolmogorov (JMAK) law is applied to describe the austenitisation, the tempering and the phase composition from austenite, ferrite, perlite and bainite. The Koistinen Marburger (KM) law is applied to describe the austenite martensite transformation and for melting and solidification. During the materials simulation with JMatPro® the phase transformation is calculated for different cooling rates (CCT) and holding temperatures (IT). DynaWeld maps the consistent information and calibrates the JMAK and KM parameters for the FEM material card.

4 Simulation model setup with DynaWeld®

DynaWeld® [8, 9] is a pre-processor tailored for welding and heat treatment tasks and supports the LS-DYNA® code which is required to run the simulation. The input is driven by the process data. The user comes into contact with the FEM code settings as less as possible. A Welding process can be combined with heat treatment in one simulation model. Figure 6 shows the main frame of the graphical user interface.

Fig.6: DynaWeld® preprocessor for welding and heat treatment

5 Example axle and gear

An axle gear component is chosen to demonstrate the capability of coupled simulation material - welding - heat treatment. Two materials are considered: a general steel with 0.11 % C, 0.45 % Mn, 1.52 % Cr and 3.30 % Ni and a cast steel for pressure purposes 10CrMoV with 0.1 % C, 0.50 % Mn, 10.2 % Cr and 0.55 % Ni. Figure 7 gives an overview of the specimen, the process steps and the thermal cycle induced by these steps: Preheating - Welding - Hardening - Tempering. The heating is simulated by heat transfer at surface and takes into account the temperature increase from surface to kernel. During quenching the diving into the quenching media is considered.

The microstructure changes during the entire process chain of welding causes temperature fields with high gradients in space and time. The heat is locally concentrated. This leads to local change of material and microstructure near the weld and to high residual stresses. During heat treatment processes the temperature distribution is more homogeneous although temperature gradients between the surface and center of parts appear. After homogeneous temperature is reached the martensite from the weld as well as the rest of the part transforms to austenite and moreover the residual stresses dissolve. The quenching process causes martensite formation and new residual stresses. During tempering the martensite transforms to tempered martensite with a shift of residual stresses (figure 8). The entire material change is directly influenced by the alloy and its proportions. Figure 9 shows the equivalent stress (Mises), figure 10 the yield stress and figure 11 the scalar of the distortion after tempering, which is the last process. The results for general steel are quite different from the results for cast steel but the manufacturing process is exactly the same. Only the difference of the chemical composition of the material - its properties predicted by materials simulation - impacts the variance in the result.
Process steps:
1) 0 s - 60 s: Preheating
2) 61 s - 63 s: Welding
3) 63 s - 800 s: Cooling at air
4) 800 s - 7000 s: Heating - austinitisation
5) 7000 s - 7500 s: Quenching in Oil
6) 7500 s - 10000 s: Cooling at air
7) 10000 s - 15000 s: Heating - tempering
8) 15000 s - 20000 s: Cooling at air

Fig.7: Process steps of example gear axle

Fig.8: Effective stress (v. Mises) during the processes for 10CrMoV

Fig.9: Result of equivalent stress
6 Summary

In welding and heat treatment processes the interaction of process model and material model has to be considered.

Materials information from materials simulation using JMatPro® and EDA® are used to create specific material cards for welding and heat treatment simulation.

MatPlusHQ as well as DynaWeld® are using these data so that they can provide solutions for the entire simulation chain material simulation ←→ process simulation for welding and heat treatment.

A focus has been put on usability and performance so that the systems can easily be used in industrial practice for design and optimisation of products and processes.
7 Literature


