DFG project Schm 746/248-1:

Integrative material and process model for the correlation of phase morphology and flow behavior of spheroidization annealed low-alloyed carbon steels "

Objectives:

Establishing Process–Microstructure–Property relationships are essential in leveraging experiment and simulation to reduce the time and cost needed to develop new materials or to improve existing materials Figure 1 illustrates how different parameters can interact leading to the mechanical properties of spheroidization annealed low-alloyed carbon steel. The spheroidization process with different parameters (e.g., temperature, holding time and constant external tension loading during the process) influences the microstructure of the steel. The resulting microstructure, in turn, has significant effects on the macroscopic mechanical properties of the material. The combination of experimental work (yellow boxes in Figure 1) and simulation methods (green boxes in Figure 1) can help to provide a deeper understanding of these interactions and to achieve the required improvement of mechanical properties.

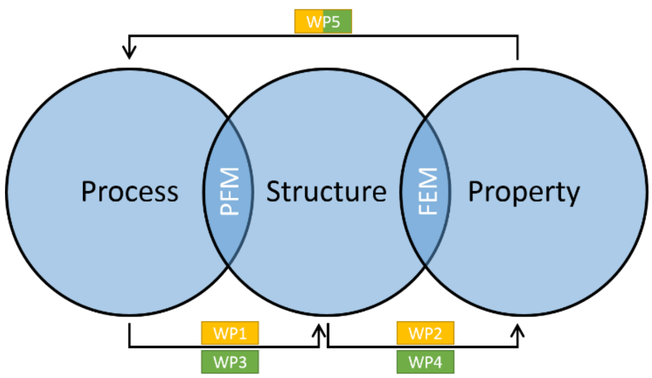


***Figure 1**: The cycle of Process-Microstructure-Property for spheroidization annealing*

The goal of this proposal is to construct a numerical model, which enables the systematic investigation of mechanical performance based on the microstructure of Fe-C alloy and which clarifies the relationship between the microstructure and the mechanical properties of steels on the micro- and macroscopic scales with a high accuracy for the development of new steels or new or improved heat treatment procedures. Special consideration should be devoted to the question of early damage due to the presence of cementite particle depending on their morphology and the local stress state.
To implement the scope and complexity of the proposed Task, a methodological approach is proposed for interdisciplinary cooperation involving two complementary research institutes: the IMF as an institute with a focus on materials and technology development for metal forming and the IMWF as an institute with recognized research experience in the field of micromechanical model development and FE simulation. The IMF is responsible for the preparation of samples of different chemical compositions, the performance of experimental heat treatments and subsequent deformation tests under various conditions as well as characterization of mechanical and technological properties. The IMWF is responsible for two- and three-dimensional microstructural characterization, determination of individual phase properties as well as the simulation based on the phase field method (PFM) and finite element method (FEM). These two institutes work closely together and complement each other's Tasks in close cooperation throughout the project period.

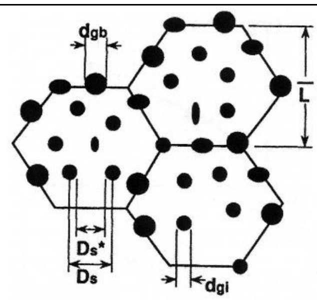
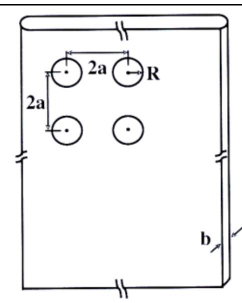
Procedure

An Fe-1C binary alloy and two Fe-1C-1.5X (X=Cr, Mo) ternary alloys are intended for the project as model material. The choice of material is based on three fundamental reasons; Firstly, high-carbon steels are very important in fabricating of parts for automobiles, industrial machines and machining tools. On the other hand, in the production of this steel group the spheroidization heat treatment is crucial to guarantee the formability and quality of products. Third, the effect of alloying elements with promoted (e.g., Cr) and retarded (e.g., Mo) impact on mechanical properties will be examined on the spheroidization kinetic of the basic chemical composition. In the project, the intercritical spheroidization is considered. The choice of this annealing type is based on the results of the own preparatory work, which determined this kind of annealing as the most economical variant.

In the first phase, by means of the PFM and FEM, the prediction of the microstructural formation in an arbitrary heat treatment process under the special influence of the alloying elements Cr, Mn and Mo on the dissolution and coagulation behavior of cementite will be modeled. At the same time, the results of the simulation will be validated with experimental findings. The produced and heat-treated specimens will be subjected to a microstructural characterization of the 2D and 3D cementite morphology. For this purpose, images will be extracted from the 2D SEM sand 3D PCT, measured with the well-known relationships from the literature (see Table 1) and compared with the results of the PFM simulations.

Subsequently, mechanical laboratory tests (e.g., tension, compression, torsion and combined loading) will be carried out on the predefined material states up to different loading stages of the test. This enables the generation of local stress conditions in the vicinity of the cementite phase with different morphologies in relation to the damage behavior of the material.

Table 1*: Microstructural parameters to be used in the proposal*

2D characterization	**3D characterization**
 [Syn94]	 [Wan10]
$\left(\frac{2}{3f}\right)^{1/2} \cdot d \cdot (1-f)$ (9) $\left(\frac{3}{2}\right)^{1/2} \cdot d \cdot \left\{\left[\frac{\pi}{4 \cdot f}\right]^{1/2} - 1\right\}$ (10) $\frac{2 \cdot d}{3 \cdot f} \cdot (1-f)$ (11) re *f* - cementite content, *d* - mean cementite particle neter, λ - the mean free ferrite path.	$\frac{a}{b} \geq 0$ (12) $\frac{a}{R} \geq 1$ (13) $\frac{R'}{R} = \frac{nR'}{kb} \leq n$ (14) $\left(\frac{4n^2-\pi}{4n^2-m^2\pi}\right) b$ (15) $\frac{a}{b_0}\left(1-\frac{\pi}{4n^2}\right)$ (16) re *k*, *m* and *n* – variables, *2a* - horizontal and vertical distance veen the centers of the holes, *b* - the original thickness of a entite lamella, *R* - radius of the circular hole before growth, radius of the circular hole after growth.

The tests on cylindrical specimens are performed only at room temperature. Comprehensive 2D and exemplary 3D microstructure analyses can then be used to make precise predictions about the microscopic behavior of cementite and its environment under mechanical stress and to clarify the deformation and damage behavior within and around cementite particle. The FEM simulation, which complements the laboratory tests, provides the correlation between the various loading conditions, local stress and strain behavior and the formability of the investigated material volume. In addition, small specimens with appropriately prepared surfaces will also be subjected to in-situ tensile or shear loading under a scanning electron microscope in order to directly observe the initiation and propagation of the local damage at cementite particle.

In the second phase, based on the relationships obtained between the applied loads and the damage behavior of cementite and its environment, the local deformation and damage evolution will be simulated by FEM. Two different fracture strain damage models are generated as analytical and mathematical fracture strain damage models. The numerical simulations are carried out with the generated fracture strain definition. The parameters of analytical fracture locus are calibrated by considering all data points (fracture strain and weighted stress state values) obtained in numerical simulations of tests. As the second approach,

the mathematical fracture strain surface based on the bi-harmonic spline method is generated. In this approach, a fracture strain surface is produced by local fracture strain in different specimens with different triaxiality and lode angle parameters. Both approaches are hybrid methods in combining numerical simulations with experimental results. The experimental global force-displacement responses are used as a reference for the numerical simulations. Numerical simulations are carried out to determine the numerical global force-displacement responses and the components of stress and strain tensors. Material ductility (i.e., fracture strain) and two stress state parameters, stress triaxiality and Lode angle parameter are calculated from strain and stress tensors, respectively. Numerical simulations are carried out with isotropic J2-plasticity. In this project, the first approach to model damage will be applied for the prediction of specimen behavior under complex loading condition.
Micromechanical models will be applied to predict the macro-mechanical behavior and micro-mechanical damage mechanisms. In order to perform micro-mechanical modelling, sufficient number of images from the microstructures should be extracted. Then the flow curves for ferrite and cementite phases have to be calculated.
Micromechanical modelling without damage can predict the macro-mechanical stress-strain curve until necking. So in order to model the damage on a microscale, the aforementioned approaches will be employed for the ferrite phase and hence failure in the cementite phase will be disregarded. The damage parameters for ferrite phase will be calibrated by macro tests as first approach. Finally, the damage scenario will be validated by in-situ test results and then applied for prediction of damage initiation and damage propagation scenario in different loading conditions. On this basis, a correlation between the determined damage behavior of the material and the loading condition will be established. This enables the prediction of a wide range of relevant load paths. In the third phase of the project, neural networks-based machine learning will be applied. Critically identified load paths from the PF and FE simulations of different cementite morphologies (e.g., shapes, sizes, orientations, possibly groupings of cementite particle, etc.) will be used as an input and to train the mechanical behavior of arbitrary steel after spheriodization heat treatment (e.g., yield stress, ultimate stress, the fracture strain in different stress states) will be predicted. The predicted data will be utilized to calibrate the damage model parameters. The validation of the determined correlations in the praxis-oriented scale for the transverse extrusion test will be carried out in the final step experimentally.

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