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CONSTITUTIVE MODELING OF STEEL WITH TEXTURE CHARACTERISTICS

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Abstract. *The optimal utilization of modern steels for building industry requires the description of microscopic constitution of these materials. The disparity in the quantity of their macroscopic properties (e.g. Youngs modulus, yield strength, ultimate strength, ductility) is purposely changed by means of microscopic constitutive differences. The hierarchical multiscale approaches give an opportunity to extend the phenomenological material description of macroscopic scale by means of microscopic information. This paper introduces an enrichment multiscale approach applicable for textured steel materials, typically occurring in hot rolled members or welded joints. Hence, texture is manifested in crystalline materials as a regular crystallographic structure and crystallite orientation, influencing macroscopic material properties. The grain texture has been described on a mesoscopic scale (μm) according to a RVE-approach and coupled with macroscopic constitutive relations by means of homogenization. On both spatial scales material has been taken into account as a continuum. The influence of manufacturing and fabrication has been incorporated into the macroscopic material description by a local grain size function. The approach has been developed for structures under static loading underlaying macroscopically elastic material responses.*

1 INTRODUCTION

Modern manufacturing technologies allow an optimal and purpose-oriented utilization of steel materials in the building industry. Thereby, the desired metallurgical constitution is created by obtaining a particular microscopic state, since all material phenomena, affecting the behavior of the structure, rely on physical effects which interact in different spatial scales from subatomic to microscopic and macroscopic range. One of early beginnings of research of this particular issue can be dated to the end of 19th century [10]. In the first half of 20th century, different approaches of homogenization methods were developed by [4][9][5][1]. These coupling approaches are oriented on transferring the results and informations obtained on lower spatial scales to the macroscopic scale. Since then, the micromechanical modelling techniques have been developing rapidly, since they are applicable in a wide range of research fields, such as mechanical engineering, biomechanics, electronics, etc. This regards mostly the application to new materials with limited number of alloys and a certain degree of similarity in microstructural constitution. Since steel materials vary in their microscopic constitution, this prospective approach can be find rarely in the field of structural steel engineering. In the context of civil engineering, all steel materials are generalized and described qualitatively by the same phenomenological material laws, differing in quantities of their properties (e.g. Youngs modulus, yield strength, ultimate strength, ductility). If the material is microscopically heterogenic and macroscopically homogeneous, it might be appropriate to use phenomenological models for civil engineering applications. This might be timesaving, but it also has limited potential to increase the reliability of the prognosis of behavior, since the material response is always closely related to microscopic state. Aside from this, these models are insufficient for steel materials with microscopic characteristics such as texture, that typically occur in hot rolled steel members or heat affected zones of welded joints. Hence, texture is manifested in crystalline materials as a regular morphological structure and crystallite orientation, that influences macroscopic material properties.

2 CONCEPTION AND METHODOLOGY

2.1 General Context

The method has been developed for materials under static loading, characterized by texture. In order to distinguish the metallurgical diversity, microscopic material law has been enriched purposely by microscopic constituents. The concerned approach will be shown on an example of a welded joint of a hot rolled ferritic/pearlitic steel, S460TM (1, a), where different microscopic states of particular zones in a narrowed area of heat affected zone and parent material are distinctive. During the manufacture of parent material (e.g. hot rolling) the grains obtained preffered cristallographic orientation. The non-randomnes of cristallographic texture reveals a macroscopic anisotropy of crystaline materials. In addition, the parent material is characterized by banded microscopical structure (1, b), which also contributes to the macroscopic anisotropy of material. The degree of anisotropy is influenced by grain size ratio in rolling direction and thickness direction (morpholgic anisotropy). The constitution of S460TM is characterized by courser bands of ferrite grains, elongated in rolling direction, and fine pearlite bands, consisting of ferrite and cementite constituents. Due to the fact that grain size and cristallographic orientation influence the macroscopic material properties, these issues will be the focus of this. The heat affected zone (HAZ) of a welded joint is a thermally and metallurgically affected area,

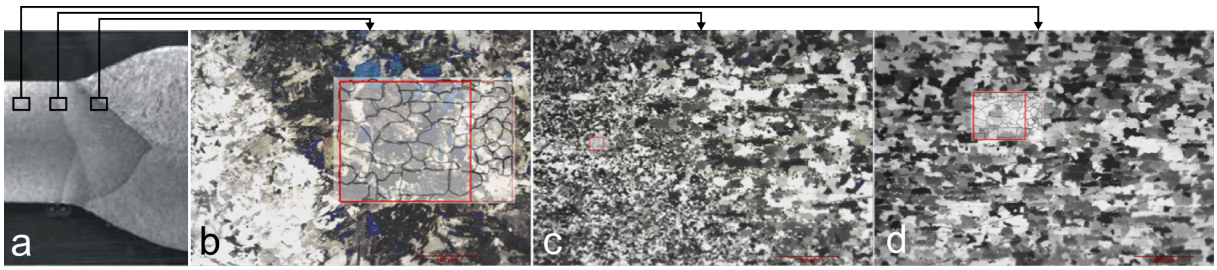

Figure 1: a) Welded joint and heat affected zone, S460TM, b) coarse grain zone, c) pearlite decomposition zone (fine grain zone), d) microstructure banding

where the initial constitution of the parent material is changed. This zone is mainly characterized by brittle and high strength constituents, martensite and bainite. The grain size varies from the course grain zone in a fusion line of a joint and a HAZ and fine grain zone in a pearlite decomposition area which is the outside margin of a HAZ (1, c and d). Every welded joint and its HAZ is unique in its structure, due to the non reproducibility of the welding process as well as inclusions, voids and microcracks. To incorporate the metallographic structure into the procedure of the response calculation of engineering structures, it is necessary to describe microscopic constitution explicitly. For this purpose, the methods of micromechanics are appropriate.

2.2 Meso-Macro Approach to Constitutive Modelling

The methodology has been derived following the principals of the micromechanical approach of the Reference Volume Element (RVE). This hierarchical multiscale method is based on the consecutive modeling of material on different spatial scales by RVE and connecting them to upper scales. Besides the scale of interest (e.g. macroscopic scale), the mesoscopic scale (μm)

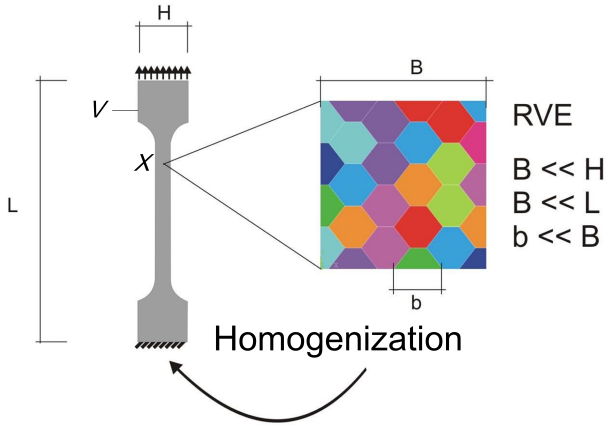

Figure 2: Principle of hierarchical multiscale approach

has been taken into account in the present example. The necessity of the description on the mesoscopic scale is given by the fact, that the constitutive parameters, which mainly influence macroscopic anisotropy of textured steels can be described on this scale. Within the context of this approach, on the macroscopic scale, body V consists of a set of infinitesimal material points X. The material point $X \in V$ has to be constitutively and geometrically described on

the lower scale (meso scale), thus demanding representativity. The models on the considered spatial scales are coupled by means of homogenization techniques to derive the mechanical relation between the microscopic components and macroscopic material response. The basic principle has been shown in figure 2. The original micromechanical approach is based on the demand of homogeneity of the material on the macroscopic scale. This demand retains the representativity of the RVE for every material point on the macroscopic body. The application to materials that obey particular local effects, such as in heat affected zones, has to be modified. Hence the homogeneity demand can not be met. The amendment consists of an adoptation of a grain size function (GSF), that describes the grain size as a function of position in a HAZ. Thus enables a consistent application of an RVE-concept for the presented purpose. An approximated grain size function of a HAZ of a butt welded S460TM connection is shown in 3. A multiple linear regression according to [6] has been used to identify the GSF. The measured grain sizes of an existing joint have been used as a response vector Y. The coordinates in thickness- and width-direction are represented by the input parameter matrix X. The approximation of the responce surface $\hat{Y}$ obey the following equation:

$$\hat{Y} = X\beta + e \tag{1}$$

By minimizing the vector of error term e, the regression coefficient vector β can be obtained according to [6]:

$$\frac{\delta SS_E}{\delta \beta} = 0, \;\; \hat{\beta} = (X^T X)^{-1} X^T Y \tag{2}$$

The quality of the approximation has been obtained by the coefficient of determination R^2:

$$R^2 = 1 - \frac{SS_E}{SS_T}, \; 0 \leq R^2 \leq 1 \tag{3}$$

which relates the sum of error squares SS_E and model response variance SS_T:

$$SS_E = e^T e, \;\; e = Y - \hat{Y}, \tag{4}$$

$$SS_T = (\hat{Y} - \bar{Y})^T (\hat{Y} - Y) \tag{5}$$

Within the measured area of HAZ, the calculated coefficient of determination $R^2 = 0.92$ shows a good approximation quality. The quality decreases for the prediction of the grain size outside of the approximation area ($R^2 = 0.67$). This result shows a potential to expand the input parameter set and incorporate the parameters, such as cooling time and temperature gradient, with the intention of effectively integrating the welding process into the expression of a GSF. As mentioned, material constitution on a mesoscopic scale is described by means of RVE. The material properties have been derived from material properties of a body-centered Fe-crystal (4). The orientation of grains within the RVE is assumed to be normally distributed. To relate the different cristallographic orientations to the global orientation of an RVE, a decomposed transformation of material tensor C_{pqrs} for every grain according to their Eulerian angles has been preformed. The transformed material tensor C_{ijkl} is calculated according to following equation:

$$C_{ijkl} = R_{ip} R_{jq} R_{kr} R_{ls} C_{pqrs} \tag{6}$$

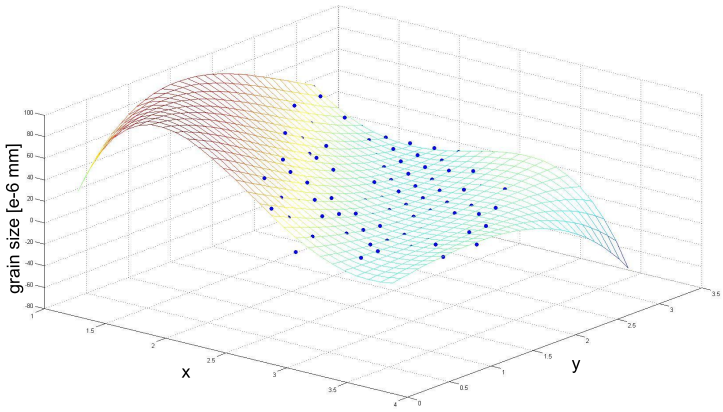

Figure 3: Approximated response curface of a GSF in a HAZ of S460TM

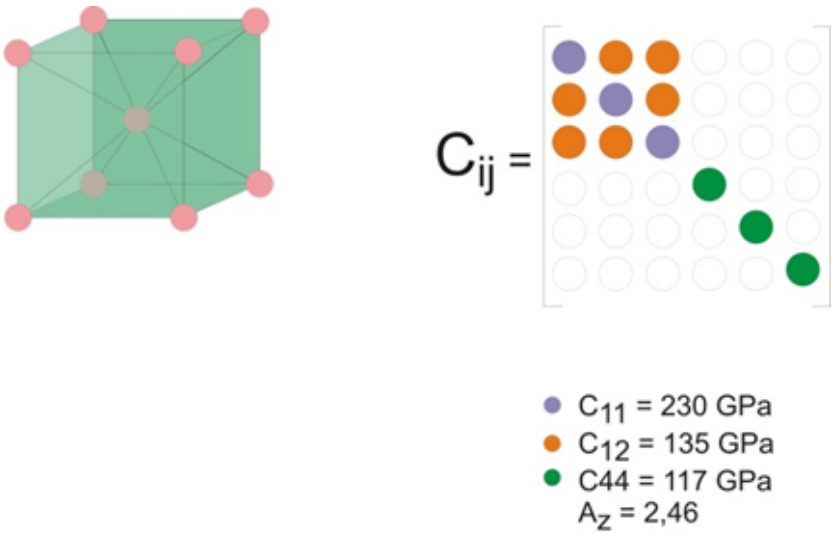

Figure 4: Material matrix of a body-centered Fe-crystal

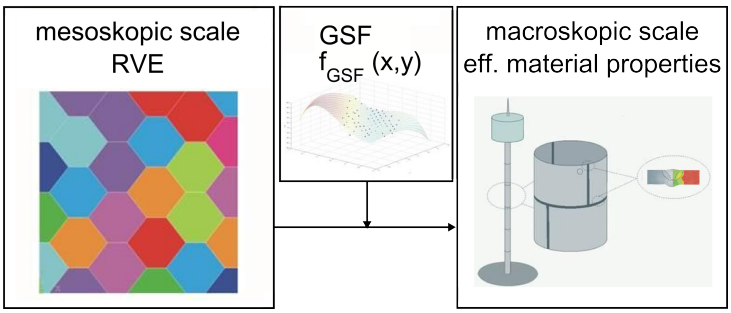

Figure 5: Principle of a meso-macro-approach

where R describes decomposed rotation matrices of three Eulerian angles [3]. To obtain effective material properties on the macroscopic scale, considering the textured structure of a mesoscale, homogenization techniques are preformed. The local strain- or stress-fields within the RVE have to be derived and homogenized over the volume [2]:

$$\langle \sigma_{makro} \rangle = \frac{1}{|V|} \int_V \sigma(x) dV, \quad \langle \epsilon_{makro} \rangle = \frac{1}{|V|} \int_V \epsilon(x) dV \tag{7}$$

The physical consistency of these approaches has been requested by equality of strain energy density on both scales:

$$\langle \sigma_{meso}(x) : \epsilon_{meso}(x) \rangle = \langle \sigma_{makro} \rangle : \langle \epsilon_{makro} \rangle \tag{8}$$

The homogenised macroscopic material tensor C^*_{ijkl} is relating the mean values of stress and strain-fields over the volume:

$$\langle \sigma_{ij} \rangle = C^*_{ijkl} : \langle \epsilon_{kl} \rangle \tag{9}$$

Within the application of the RVE-concept, periodic boundary conditions have been implemented, fulfilling the following relation [7]:

$$u^B_i i - u^A_i = \epsilon_{ij}(x^B_j - x^A_j) \tag{10}$$

where the displacement u_i of opposite boundaries A and B has been determined by means of strain ϵ_{ij} and the distance of the respective locations x_j. The application of periodic boundary condition is an RVE-concept based constraint, where all macroscopic material points, represented by RVE, obey identical behavior on their opposite boundaries. For the calculation of all components of the macroscopic material tensor, six uniform loading conditions of the RVE are necessary: three axial strains and three sher strains. With the presented approches and assumptions, an exemplary method has been derived, which incorporates the metallurgical material state into the constitutive material model used for calculation of response of steel structures. In figure 5, a main principle of the method is shown. The first calculations of RVE are focused on identification of relevant influencing factors, to assure the representativity of the model. For this purpose, the effect of grain size, grain shape and RVE-size have been investigated. The influence of grain geometry has been performed on two-dimensional models, considering rectangular and truncated octahedral grains. The representativity of the RVE is apparent when the influence of the number of grains on the macroscopic material properties is investigated. Additional analysis has been performed on a three-dimensional model with cubic formed grains.

The deviation of RVE-models with respect to their size, has been investigated by means of an error estimate according to [8]. This error estimator is formulated as a ratio of a standard deviation of an equivalent von Mises stress and a representative equivalent von Mises stress of an RVE-model with 2744 grains:

$$err = \frac{S(\sigma_{vM})}{\sigma_{vM}^{2744}} \tag{11}$$

3 RESULTS

The size of the RVE has been investigated with respect to the derived effective Young's modulus of the macroscopic material. In addition, the grain shapes have been analysed. The results of the effective Young's modulus in the rolling direction with respect to RVE-size for rectangular and truncated octahedral grains are shown in figure 6. The derived results show

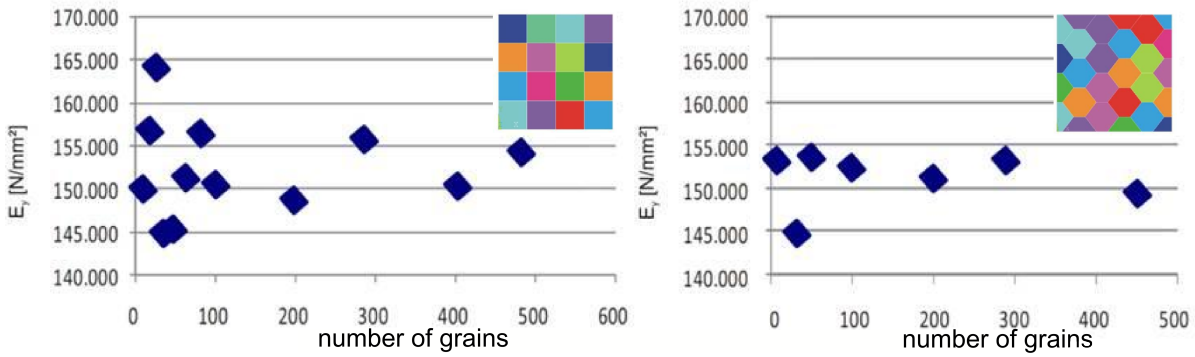

Figure 6: Influence of grain shape and RVE size on effective Young's modulus

negligible influence of grain shape on the Young's modulus on macroscopic scale. As the RVE size increases, the effect on Young's modulus decreases. The RVE-models with appr. 400 grains vary 3%. Hence, for further three dimensional investigations, a cubic grain shape has been assumed. The analysis of the error estimate according to 11, reveals asymptotic behavior, as shown in figure 7. The variation of error is insignificant for RVE with more than 1000 grains. The presented investigations create a basis for analysis of the influence of the grade of banded

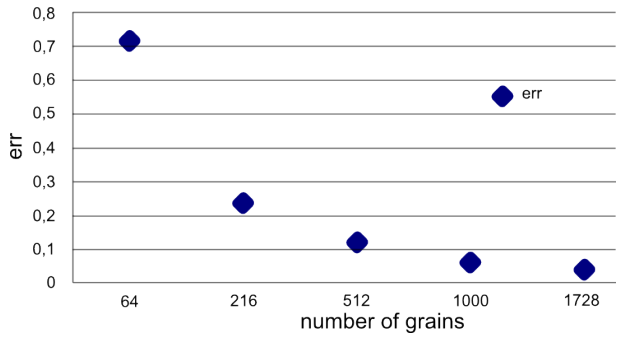

Figure 7: Error estimate based on equivalent von Mises stress for different RVE size according to equation 11

microscopic structure on the anisotropy on the macroscopic scale. The purpose of this analysis is to adaptively integrate the method into calculations on a macroscopic scale.

4 CONCLUSIONS

The proposed method enables the description of the metallurgical state of steel materials for the purpose of the analysis of structural responses in civil engineering applications. There are advantages to the possibility of including a grain size function for the specification of local effects such as heat affected zones of welded joints. The first numerical investigations show negligible influence of grain shape. The error estimation analysis, based on equivalent von Mises stress, has been used and a representative RVE-size have been derived. An outlook for the next investigations has been given. With the presented methodology, a first step has been taken towards a new basis of calculation, as well as an effective design procedure for steel structures.

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