An Eshelby inclusion based model for cementite variants in hypereutectoid steel

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Abstract

A multiscale homogenization model has been developed for the description of the elastic properties of hypereutectoid pearlitic steels with proeutectoid grain boundary cementite precipitates through the calculation of their stiffness matrix. This model is based on the Eshelby inclusion problem [1]. Different microstructural cases are tested: a lamellar versus spheroidized structure of the pearlite, and the presence of a continuous versus discontinuous layer of proeutectoid cementite around the pearlite grains. Depending on the case, Benveniste's approach of the Mori-Tanaka method [2] or classical or generalized self-consistent calculation schemes [3, 4] have been used. Employing elastic moduli of the pearlitic ferrite, the pearlitic cementite and of the proeutectoid cementite, together with the volume fraction of each of these phases, a two steps homogenization calculation is conducted, 1) the determination of the stiffness matrix of the pearlite grains followed by 2) the determination of the homogenized stiffness matrix of the metal sample. The diversity of lamellar pearlite grain orientations can be considered in our model. Tentative results regarding the coefficients of the homogenized stiffness matrix are quite encouraging when compared to the literature. By coupling with thermokinetic phase transformation simulations this new application of the Eshelby model allows for a fast prediction of the elastic properties of hypereutectoid steel with diversity of pearlitic microstructures.

Construction of a multiscale Eshelby model

The probed microstructure consists of pearlite colonies with proeutectoid cementite precipitates forming a continuous or discontinuous layer around the austenite grain boundaries. First the stiffness matrix of a pearlite colony is calculated. If the pearlite is spheroidized, Benveniste's approach of the Mori-Tanaka method is used with spherical cementite inclusions inside a ferritic matrix [2]. If the pearlite is lamellar, a classical self-consistent scheme with an aggregate of cylindrical lamellae of cementite and ferrite is used [3], and the resulting stiffness matrix is homogenized by taking into account a fixed diversity of grain orientations. Then the stiffness matrix of the final material with spherical pearlite colonies is calculated. A generalized self-consistent scheme [4] has to be used if the proeutectoid cementite is forming a continuous layer on the grain boundaries, and a classical self-consistent scheme [3] is used if the proeutectoid cementite is discontinuous. The cementite precipitates are in this case treated as spherical.

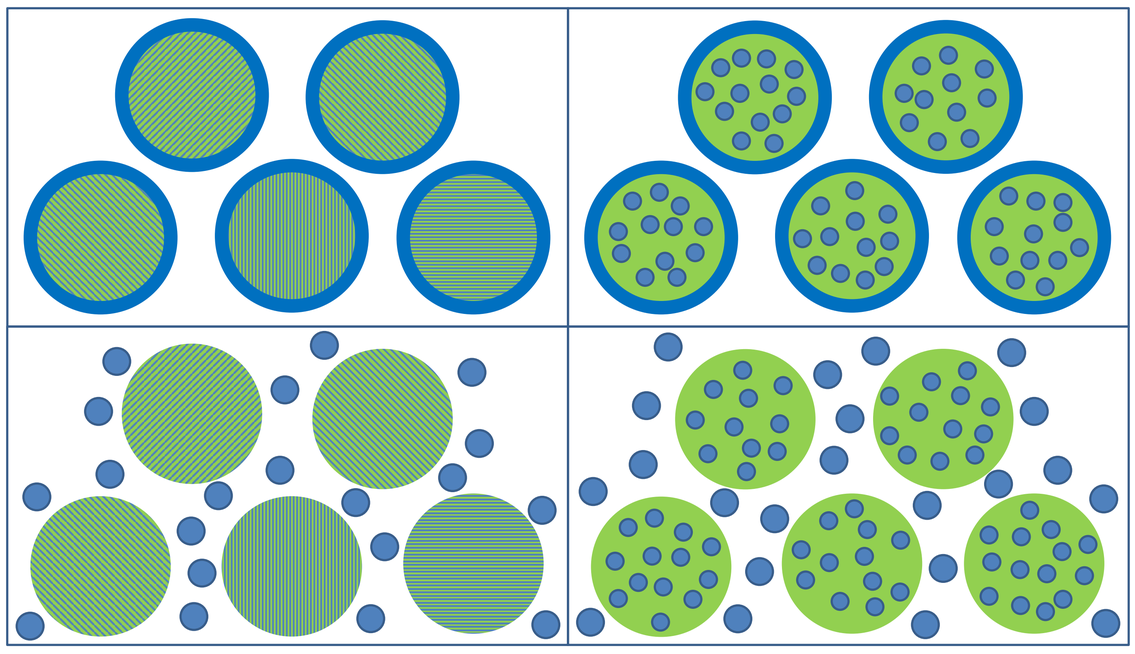

Figure 1: Schematic view of the modelling of the microstructure. Cementite is shown in blue, ferrite is shown in green. Left: lamellar pearlite. Right: spheroidized pearlite. Up: continuous grain boundary cementite. Bottom: discontinuous grain boundary cementite.

Evaluation of elastic parameters

The stiffness matrix of the homogenized material and the associated elastic moduli are evaluated from input data found in the literature considering both ferrite and cementite as isotropic materials. The standard deviation of the different material data found in the literature for ferrite is much smaller [5] than the one for cementite [6]. For this reason, only one set of material data for ferrite has been used and Young's modulus calculation results have been compared for several different material input datasets for cementite [6, 7, 8]. The effects of microstructural parameters have also been investigated: proeutectoid cementite thickness, pearlite lamellae slenderness ratio (length/width).

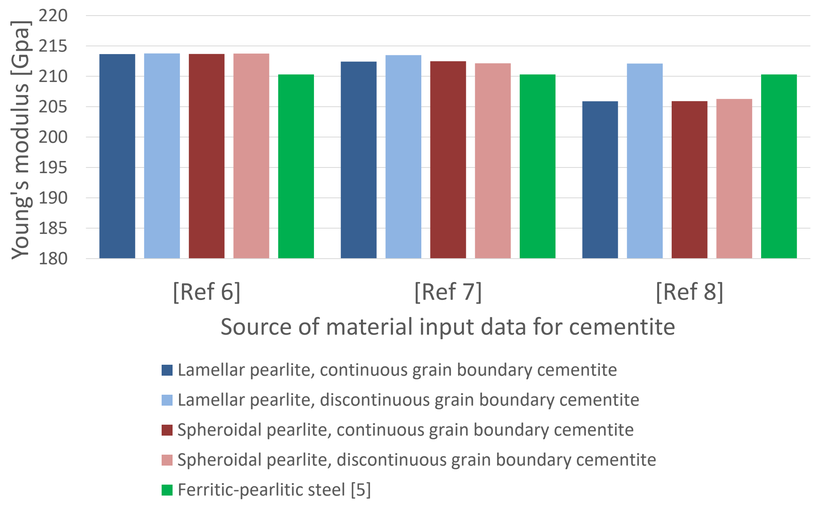

Figure 2: Calculated Young's modulus with the 4 different types of models, with material input data for ferrite from [5] and with material input data for cementite from [6, 7, 8], compared to the Young's modulus for ferritic-pearlitic steel from [5]. Microstructural parameters: proeutectoid cementite thickness = 0,3 µm ; when pearlite lamellar: lamellae slenderness ratio = 50

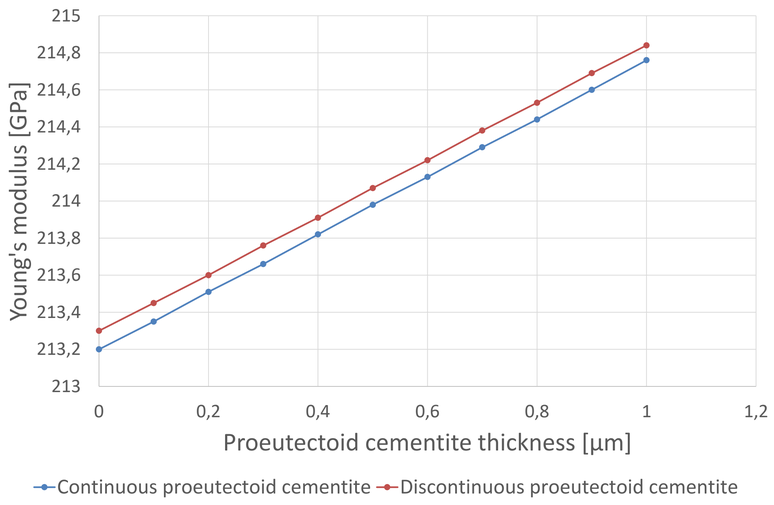

Figure 3: Calculated Young's modulus as a function of the proeutectoid cementite thickness from the models with lamellar pearlite and continuous or discontinuous proeutectoid cementite. Pearlite lamellae slenderness ratio = 50 ; material input data for ferrite: [5] ; material input data for cementite: [6]

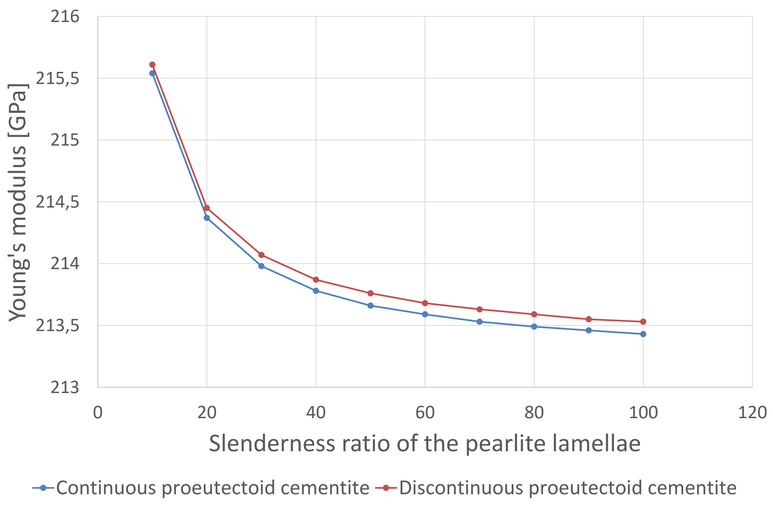

Figure 4: Calculated Young's modulus as a function of the pearlite lamellae slenderness ratio from the models with lamellar pearlite and continuous or discontinuous proeutectoid cementite. Proeutectoid cementite thickness = 0,3 µm ; material input data for ferrite: [5] ; material input data for cementite: [6]

Summary

- All our results are close to the data found in the literature.
- Despite the variations in the input data for cementite, there is only a small variation in the homogenized material's Young's modulus. This may be explained by the small volume fraction of cementite in the material.
- The modelled effect of the proeutectoid cementite thickness and of the pearlitic lamellae shape on the elastic properties of the material is small compared to the values of the calculated Young's moduli. This was expected since these microstructural artefacts are particularly effective beyond the elastic domain.
- Application of our approach to the modelling of plasticity is on the way.

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