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Original Contributions

M. Vogric, E. Povoden-Karadeniz: A multiscale mean field model for elastic properties of hypereutectoid steels

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A multiscale mean field model for elastic properties of hypereutectoid pearlitic steels with different microstructures

Multiscale modeling of macroscopic elastic properties of pearlitic hypereutectoid steel using the Eshelby matrix-inclusion approach is possible. The model works through successive homogenization steps, based on the elastic properties of cementite and ferrite. Globular pearlite is homogenized using a Mori-Tanaka approach. Lamellar pearlite and pearlite colonies with fragmented proeutectoid cementite are homogenized by a classical self-consistent scheme. In the case of pearlite colonies surrounded by a continuous cementite film, a generalized self-consistent scheme is used. The influence of microstructural parameters such as the pearlite colony size or the thickness of the proeutectoid cementite on Young's and shear moduli and on coefficients of the stiffness tensor is simulated. Proof of concept is obtained by comparison between predicted elastic behavior and experimental results from the literature.

Keywords: Micromechanics; Multiscale; Homogenization; Hypereutectoid; Steel

1. Introduction

The elastic properties of a material depend on its microstructure. In continuum micromechanics modeling, a microstructure is defined as the whole of inhomogeneities in a given material at a given state. Inhomogeneities can be classified by their dimension from 0D, for example a lattice vacancy, up to 3D, including spatially distributed phases and their different chemical compositions, crystallographic structures and intrinsic elastic properties. A microstructure evolves during thermo-mechanical treatment. Each transient state of an evolving microstructure during thermo-mechanical treatment can be defined in terms of the changes of microstructural constituents such as grain and subgrain size and orientation distribution, as well as phase contents, sizes and morphologies. The evolving microstructure affects the macroscopic materials properties. These effects of micro- or mesoscale artefacts on the macroscopic elastic properties of the material can be described by continuum micromechanics modeling. A simple mean field approach simulates these properties for the material taken as a homogeneous bulk. For the critical issue of the transition from the microscale to the macroscale, established homogenization models are employed in a multiscale approach. This means, as in Hellmich's group's work [1-4], that successive homogenizations are applied at different size scales. We use homogenized phases at lower scales as input for homogenization at higher scales. The use of such a multiscale homogenization approach – as opposed to single-step homogenization - is assessed for biological or construction materials (bones, concrete...), as presented by Hellmich's group, but not for polycrystalline metals. Repeated homogenization steps are, however, required in the modeling of hypereutectoid steels due to their composite nature of pearlite and the presence of proeutectoid cementite. The assessment of the applicability of multiscale homogenization to this material is thus the innovative part of the present work. The used homogenization models are based on Eshelby's equivalent inclusion method [5] and are well documented in the literature [1, 6, 7]. Up to now, their use in steel modeling has been restricted to microstructures requiring only a single homogenization step. Examples include the simulation of the elastoplastic properties of dual-phase steels by Brassart [8] with adapted Hill's self-consistent schemes [9], simulative strength-ductility optimization of transformation-induced plasticity steels and associated phase stability criteria by Lani [10] using a Mori-Tanaka homogenization scheme [11] combined with the secant pseudo-elastic moduli from Berveiller and Zaoui [12], and the evaluation of elastoplasticity of a dual-phase steel by Perdahcıoğlu [13], comparing the results of different adaptations of Hill's homogenization schemes [9]. The focus will be kept on elastic properties in the present work, since its purpose is to evaluate the validity of the adaptation of multiscale homogenization for the complex microstructures of hypereutectoid steel.

2. Material

Hypereutectoid steels contain a carbon concentration above the carbon concentration for the eutectoid decomposition from austenite to ferrite (α) and cementite (Fe₃C, θ), which, in the Fe-C system, lies at 0.77 wt.% C. Their higher hardness in comparison to steels with lower carbon concentrations makes them particularly interesting for some industrial applications such as rail production. During the cooling involved in the alloy's production process after the austenitization, proeutectoid cementite (or, synonymous, secondary cementite, denoted as θ_{S} in the following) nucleates at the austenite grain boundary edges and corners [14] and may form a continuous film (CC) or fragmented film (FC) along the grain boundary [15]. Once the temperature of the alloy is below the steel eutectoid temperature, the eutectoid reaction starts, and pearlite colonies with alternating lamellae of $\alpha_{\rm P}$ and $\theta_{\rm P}$ [16] grow from the austenite grain boundaries. Due to the effect of carbides formed prior to pearlite [17] or as a consequence of soft annealing [18], the pearlite may be spheroidized. In this case, in place of a lamellar pearlite (LP) microstructure, globular pearlite (GP) is found, which consists of θ precipitates within a matrix of α .

3. Multiscale mean field continuum micromechanics modeling

In our present modeling, macroscopic mechanical properties of hypereutectoid steel are deduced from the knowledge of the mechanical properties of the individual phases composing this material, i.e. proeutectoid cementite θ_S , pearlitic cementite (θ_P) and pearlitic ferrite (α_P). The key idea of the present model is that the investigated material follows the so-called Eshelby matrix–inclusion problem [5]: the sample can be considered as a composite material made of a matrix surrounding ellipsoidal inclusions. Consistent modeling requires consideration of interactions between the different inclusions. For this, different calculation schemes are used, the Mori-Tanaka, classical self-consistent scheme (CSCS) and the generalized self-consistent scheme (GSCS). In essence, a virtual reconstruction of various hypereutectoid steel microstructures is obtained by our model, and their respective elastic properties can be evaluated. Integral parts of the model development are presented in the following.

3.1. Multiscale homogenization

Homogenization is defined as the replacement of a heterogeneous material by an equivalent statistically homogeneous one, having the same macroscopic behavior and described by a representative volume element (RVE). Here, the RVE is treated as the smallest material volume element for which the macroscopic behavior of the *constitutive moduli* of the homogenized material are a sufficiently accurate approximation of the macroscopic mean field response of the same moduli in the microheterogeneous material [19]. The separation of scales implies

$$L \gg d$$
 (1)

where *L* is the characteristic length of the RVE and *d* is the characteristic length of the inhomogeneities within the RVE. This separation of scales is a limiting factor defining a maximal size scale for the inhomogeneities compared to the RVE. It appears that L = 4.5d is sufficient to guarantee a high accuracy of the results, with a maximum error of 1% [19]. Within one RVE a set of homogeneous or quasihomogeneous subdomains can be defined, which are called material phases [20].

In a multiscale approach, a previously defined material phase that appears quasi-homogeneous on the scale of the RVE may still exhibit a heterogeneous internal microstructure when observed at its own characteristic scale. We may then define a new RVE of smaller dimensions (typically of the same size scale as the inhomogeneities in the larger RVE), representative of respective material phase and apply the rule of separation of scales as defined by Eq. (1), for the new RVE [3]. Then it is possible to obtain iteratively the macroscopic properties of the entire material from the properties of the smallest identified material phases constituting the macroscopic material. The scale of the smallest material phase involved in the model is confined by the usability of continuum mechanics. This effectively allows taking into account phases with a size in the order of magnitude of 100 nm [3].

3.2. Linear elasticity and the homogenization problem

Typically, metallic materials show linear elastic behavior. We thus only consider linear elasticity. We consider an RVE of domain Ω and volume V, and we set the following constitute equations: Hooke's law for linear elasticity (Eq. (2)), static equilibrium conditions disregarding volume forces (Eq. (3)), and linear strain–displacement relations (Eq. (4)).

$$\sigma(\underline{x}) = C(\underline{x}) : \varepsilon(\underline{x})$$
(2)

$$\operatorname{div}\,\sigma(\underline{x}) = 0\tag{3}$$

$$\varepsilon(\underline{x}) = \frac{1}{2} (\nabla \underline{u} + {}^{t} \nabla \underline{u})$$
(4)

Here, x is the position vector, $\sigma(x)$ and $\varepsilon(x)$ are respectively the second-order tensors for the local stresses and strains, C(x) is the fourth-order stiffness tensor, and u(x) is the displacement tensor. The double dot ":" notes the double contraction tensor product, such that for example for Eq. (2) $\sigma_{ii} = C_{iikl} \varepsilon_{kl}$. The so-called *concentration* or *localization* problem in continuum micromechanics is concerned with the modeling and derivation of the local stress and strain fields from the knowledge of the macroscopic stress and strain fields $\Sigma(X)$ and E(X), respectively. The homogeniza*tion* problem on the other hand is concerned with the derivation of the macroscopic stress and strain fields from the knowledge of the local ones. As explained originally by Zaoui [6] and resumed by the research group of Hellmich [1, 3, 20, 21], the original localization problem requires setting of detailed boundary conditions, which is why homogeneous macroscopic strain boundary conditions - or socalled Hashin boundary conditions [22] - are assumed:

$$\underline{u}(\underline{x}) = E \underline{x} \tag{5}$$

and under such homogeneous strain boundary conditions, the following strain average rule follows:

$$E = \frac{1}{\Omega} \int_{\Omega} \varepsilon(\underline{x}) \mathrm{d}V \tag{6}$$

And similarly, stress averaging on the macroscopic scale inside the RVE leads to:

$$\Sigma = \frac{1}{\Omega} \int_{\Omega} \sigma(\underline{x}) \mathrm{d}V \tag{7}$$

The macroscopic stress and strain fields, $\Sigma(\underline{X})$ and $E(\underline{X})$, are now defined as spatial macroscopic average stresses Σ and strains E. Meanwhile, from the point of view of the homogenization problem, we write:

$$\Sigma = \sum_{p} f_{p} \sigma_{p} \tag{8}$$

$$E = \sum_{p} f_{p} \varepsilon_{p} \tag{9}$$

where p is an index running over all phases considered in the RVE, f_p is the volume fraction of phase p, and σ_p and ε_p are the second-order tensors of average phase stresses and strains for the phase p, respectively. For the complete description of the multiscale problem a localization relation is needed, allowing to reach every individual σ_p and ε_p from respectively Σ and E. The linearity of the constitutive equations (Eqs. (2) to (4)) and the unicity of their solution leads to the definition of the fourth-order strain concentration tensors of phase p, A_p , with:

$$\varepsilon_p = A_p : E \tag{10}$$

We finally distinguish a macroscopic stiffness tensor C^{hom} and a phase stiffness tensor C_p for the phase p allowing the use of the macroscopic Hooke's law for linear elasticity and the same constitutive law as given by Eq. (2) but for phase p:

$$\Sigma = C^{\text{hom}} : E \tag{11}$$

$$\sigma_p = C_p : \varepsilon_p \tag{12}$$

 C^{hom} is derived from the different phase stiffness tensors and the previous relations as shown in Hellmich's group's works [2, 4], considering that f_p and C_p are supposed to be known for each phase p and that A_p can be estimated using matrix-inclusion calculations such as presented by Eshelby [5] and Benveniste [23]:

$$C^{\text{hom}} = \sum_{p} f_p C_p : A_p \tag{13}$$

and finally:

$$C^{\text{hom}} = \sum_{p} f_{p}C_{p} : \left[I + P_{p}^{0} : (C_{p} - C^{0})\right]^{-1}$$

$$: \left\{\sum_{q} f_{q} \left[I + P_{q}^{0} : (C_{q} - C^{0})\right]^{-1}\right\}^{-1}$$
(14)

where I is the fourth-order identity tensor, P_p^0 is the fourthorder Hill tensor accounting for the shape of the phase pforming an inclusion within a matrix described by the fourth-order stiffness tensor C^0 . C^0 is the stiffness tensor of a homogeneous matrix of an Eshelby matrix-inclusion configuration. Its calculation schemes are discussed in the following.

3.3. Parametrization of the Eshelby matrix–inclusion problem

The material RVE is homogenized by considering it as an Eshelby matrix-inclusion configuration, a composite with a set of ellipsoidal inclusions embedded in a homogeneous matrix. The calculation schemes used in the present work for the determination of C^0 are the following: the Mori-Tanaka calculation scheme [11] as reformulated by Benveniste [23], recommended for the homogenization of real matrix-inclusion composites; the CSCS [24–26], recom-

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mended for polycrystalline aggregate structures; and the GSCS [27, 28] for a polycrystalline aggregate in which every individual inclusion is surrounded by a film of a homogeneous matrix phase. We used the more recent formulation by Benveniste of GSCS in this work [28]. This formulation requires isotropic elastic behavior of the inclusions and the film, and all inclusions have to be spherical.

The derivation method of the Hill tensor (Eq. (14)) depends on the C^0 tensor, on the possible stiffness symmetries and, in the case of an ellipsoidal inclusion, on the aspect ratio *a* and the slenderness ratio *s* of the inclusion,

$$a = \frac{r_1}{r_2} \text{ and } s = \frac{r_1}{r_3}$$
 (15)

where r_i is the length of the inclusion in the direction *i* of the system's orthogonal coordinate system attached to the inclusion. The direction i = 3 will be preferentially given to

the direction of the longest inclusion dimension. For further details about the derivation of Hill tensors, the reader is referred to the literature [3, 6].

3.4. Implementation of tensor calculation

Theory of continuum micromechanics is built via tensor calculation, computed by a simpler matrix formulation. The different tensors involved in our work are fourth-order tensors with symmetry rules allowing reduction of the original 81 coefficients of the tensor to 36 distinct components. The Mandel or Kelvin–Mandel variant of the Voigt notation is used for equivalence between tensor operations and matrix operations, as presented and discussed in [29–31]. With *i*, *j*, *k* and *l* being the indexes of the coefficients C_{ijkl} in the considered fourth-order stiffness tensor:



Fig. 1. Schematic representation of the real microstructure, with cementite (black) and ferrite (white) (left side) and the different steps of the multiscale modeling approach. σ_a = uniform far-field stress; $\sigma^{(m)}$ = effective matrix stress. h.p. = homogenized pearlite; h.i.p. = homogenized isotropic pearlite.

Table 1. Homogenization schemes used for studied microstructures.

	Case 1	Case 2	Case 3	Case 4
Steel microstructure Homogenization scheme of pearlite	LP CSCS	LP CSCS	GP Mori-Tanaka	GP Mori-Tanaka
Phase relations θ_s appearance Homogenization scheme of θ_s	Parallel discs of α and θ CC GSCS	Parallel discs of α and θ FC CSCS	θ spheres in α matrix CC GSCS	θ spheres in α matrix FC CSCS
Virtual microstructure	θ film around pearlite sphere	Pearlite spheres and θ spheres	θ film around pearlite sphere	Pearlite spheres and θ spheres

$$C = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133}\sqrt{2}C_{1132}\sqrt{2}C_{1131}\sqrt{2}C_{1121} \\ C_{2211} & C_{2222} & C_{2233}\sqrt{2}C_{2232}\sqrt{2}C_{2231}\sqrt{2}C_{2221} \\ C_{3311} & C_{3322} & C_{3333}\sqrt{2}C_{3332}\sqrt{2}C_{3331}\sqrt{2}C_{3321} \\ \sqrt{2}C_{2311}\sqrt{2}C_{2322}\sqrt{2}C_{2333} & 2C_{2332} & 2C_{2331} & 2C_{2321} \\ \sqrt{2}C_{1311}\sqrt{2}C_{1322}\sqrt{2}C_{1333} & 2C_{1332} & 2C_{1331} & 2C_{1321} \\ \sqrt{2}C_{1211}\sqrt{2}C_{1222}\sqrt{2}C_{1233} & 2C_{1233} & 2C_{1231} & 2C_{1221} \end{bmatrix}$$

$$(16)$$

This type of notation is used with all fourth-order tensors in the present work. When one knows the stiffness matrix C of a material, it is possible to obtain the Young's moduli E_i for the different directions i of the coordinate system. Isotropic behavior, for the case of GSCS, further allows for straightforward evaluation of bulk modulus κ and shear modulus μ of the material.

4. Application to microstructure modeling of hypereutectoid steel

4.1. Hypereutectoid steel microstructures and their avatars

Four microstructures of hypereutectoid steel are considered: 1) Lamellar pearlite colonies with CC (denoted LP/ CC in the following); 2) LP/FC; 3) Globular pearlite colonies (GP) with CC (GP/CC); 4) GP/FC. A schematic representation of the studied microstructures and their modeled counterparts is presented in Fig. 1, with classical definitions of stress for the homogenization schemes. Their respective homogenization schemes are listed in Table 1.

The following assumptions are used in the mean field elasticity modeling of lamellar pearlite: we consider that there is only one orientation of the pearlite lamellae per former austenite grain. The virtual microstructure then contains an ensemble of pearlite colonies with exactly the same lamellar structure but different orientations, representing one material phase per orientation, surrounded by θ_s . Indeed, by this setup, the influence of θ_s on elastic properties will be intrinsically overestimated. It should also be mentioned that an RVE cannot be perfectly filled only by spheres. This supposes a partial virtual overlapping of the spherical pearlite colonies.

The elastic properties of θ and α are sufficient inputs for the calculation of the elastic properties of the entire material. Both phases are considered as isotropic. The dependence of elastic properties on direction due to relative crystallographic orientation differences between θ_P and α_P are neglected. Orientation differences are expected to vanish at the macroscopic scale after homogenization due to the presence of multiple pearlite colonies with diverse orientations in the material. This further advises the use of simple combinations of elastic parameters, bulk and shear moduli as modeling inputs instead of full stiffness matrices.

4.2. Determination of stiffness matrix

For derivation of the stiffness matrix of the homogenized pearlite C_{pearl} for both studied pearlite types, LP and GP,

the following inputs are used: the stiffness matrix of θ C_{pcem} , the stiffness matrix of ferrite C_{fer} , the volume fraction of θ_P , f_{pcem} and the volume fraction of α_P , f_{pfer} . For LP, the thickness/length aspect ratio a_{pcem} and the slenderness ratio s_{pcem} of θ_P lamellae, and of α_P lamellae (a_{pfer} , s_{pfer}) are additional modeling inputs. We consider that the lamellae have the shape of discs parallel to directions i = 2 and i = 3 (see Table 1), therefore aspect and slenderness ratios are equal. Considering equal length – or diameter – of θ_P and α_P lamellae (l_{lam}), the following relations hold:

$$a_{\rm pcem} = s_{\rm pcem} = \frac{f_{\rm pcem}.\lambda}{l_{\rm lam}} = f_{\rm pcem}.\omega \tag{17}$$

$$a_{\rm pfer} = s_{\rm pfer} = \frac{f_{\rm pfer}.\lambda}{l_{\rm lam}} = f_{\rm pfer}.\omega$$
(18)

with

$$\omega = \frac{\lambda}{l_{\text{lam}}} \tag{19}$$

 λ is the interlamellar spacing. ω may be seen as a "generalized aspect ratio" for both types of pearlite lamellae. It describes the general trend for the aspect of both $\alpha_{\rm P}$ and $\theta_{\rm P}$ lamellae due to their length and interlamellar spacing, weighted by $f_{\rm pfer}$ and $f_{\rm pcem}$. This definition of ω allows for the setting of the lamellar shape independently of the size of the pearlite colony. In order to avoid scaling problems with lamellar inclusions of too large dimensions in comparison to the dimensions of the RVE, i. e. the size of the pearlite colony, for a given $d_{\rm pearl}$, we define a maximal pearlitic lamellar length $l_{\rm max} = d_{\rm pearl}/4.5$, resulting in the minimal general slenderness factor $\omega_{\rm min}$ for a given interlamellar spacing λ

$$\omega_{\min} = \frac{4.5\lambda}{d_{\text{pearl}}} \le \omega \tag{20}$$

The stiffness matrix of the entire homogenized material, C_{mat} is derived using C_{cem} , the previously calculated C_{pearl} , the volume fraction of θ_{S} , f_{scem} and the volume fraction of pearlite f_{pearl} . d_{scem} is the thickness of the θ_{S} layer in the case of CC, or precipitate diameter in the case of FC. An approximation of f_{scem} from d_{pearl} and d_{scem} is possible, considering the volume of a pearlite sphere relatively to the volume of a surrounding θ_{S} film of thickness $d_{\text{scem}}/2$:

$$f_{\text{scem}} = \frac{d_{\text{scem}} \cdot \left(3 \cdot \left(d_{\text{pearl}} + \frac{d_{\text{scem}}}{2}\right)^2 + \left(\frac{d_{\text{scem}}}{2}\right)^2\right)}{4 \cdot \left(d_{\text{pearl}} + d_{\text{scem}}\right)^3}$$
(21)

For FC, C_{mat} is derived using the classical self-consistent scheme. We note that for FC, Eq. (21) will overestimate f_{scem} . The lack of systematic statistically relevant data on the differences in f_{scem} between CC and FC in the literature prevents us from evaluating the exact extent of this overestimation. However, we qualitatively assume the use of Eq. (21) acceptable.

4.3. Implementation of the diversity factor

For CC, C_{mat} is derived using GSCS because it is the only homogenization scheme allowing description of a homogeneous matrix film surrounding an inclusion without breaking the rule of separation of scales. This requires a further constraint for the combination LP/CC, since the equations used for GSCS work only if all phases constituting the homogenized material are isotropic [28]: not only θ_s but also pearlite must show isotropic properties. The LP case leads only to transverse isotropy since pearlite is constituted here of parallel discs of isotropic θ_P and α_P materials. The problem is solved by inserting an intermediate step between the homogenization of the single pearlite inclusions and the homogenization of the macroscopic material. In this intermediate step, we define a diversity factor \varDelta of the pearlite colonies' orientations. The orientation of the lamellae of a given colony is defined using a set of three Euler angles, and \varDelta is an integer that represents how many different equidistant values each Euler angle is allowed to take. This means that for a given Δ , there are Δ^3 different sets of Euler angles. Once \varDelta is defined, a CSCS is used, including a set of Δ^3 pearlite colonies with the different orientations. Due to the fact that orientation distributions of pearlite colonies have not been researched yet, \varDelta is calibrated here in a way to approximate isotropic elastic properties for pearlite, and the according stiffness matrix C_{ipearl} . C_{ipearl} will then be used instead of C_{pearl} for the final homogenization step, see Fig. 1 for the case 1 (LP/CC). Finally, the homogenized macroscopic material is isotropic in the four cases LP/GP - CC/FC.

In the LP/CC case, the requirement of isotropy due to the use of GSCS prohibits the investigation of preferential pearlite colony orientations. In principle it would be possible to homogenize an anisotropic CC material considered as composite made of a θ matrix embedding a – previously homogenized by CSCS – single pearlite inclusion instead, using the Mori-Tanaka scheme, and subsequently a macroscopic aggregate of such composites could be homogenized using CSCS. In fact, this method would however break the rule of separation of scales (Eq. (1)). Fully aware of this violation, we tested its outcome in comparison to the approach with GSCS, with similar input data and similar Δ . We use Δ in this example for comparability with the results using GSCS. This analysis assisted our understanding of present modeling limitations and provided clues for our continuative modeling, as discussed in Section 6.2.

4.4. Experimental input data

Input data for the derivation of C_{cem} and C_{fer} were taken from the literature. The standard deviation of this material data found in the literature is small for α [32] but larger for θ [33]. Knowing this, we chose to test our model using data for θ only from Ledbetter [33] since this is a quite recent work on isotropic elasticity of cementite and consistent with other recent data on monocrystalline cementite [34]. Modeling results are validated by literature data for hypereutectoid steel. The simulation yields an entire stiffness matrix of ideal Fe–C hypereutectoid steel. Whereas directly comparable literature data is missing, the Young's (*E*) and shear (μ) moduli of AISI 1080 steel [35], showing an LP microstructure, are available. Further, there is information on all stiffness matrix terms for pearlitic steel with 0.82 wt.% C and a LP microstructure [36]. Other experimental data on C_{1111} are available for a hypoeutectoid ferritic–pearlitic steel with an LP microstructure [32]. Evaluation results of computed C_{1111} will be presented and compared with experimental data [32, 36]. For the evaluation of elastic and shear moduli from the virtual stiffness matrix theoretical values of f_{pcem} and f_{pfer} are calculated from the Fe–C phase diagram, i.e. $f_{pcem} = 11\%$ and $f_{pfer} = 89\%$ and inserted into Eqs. (17), (18), and (21) in order to determine a_{pcem} , a_{pfer} and f_{prem} .

order to determine a_{pcem} , a_{pfer} and f_{scem} . One word on the accuracy of the data used for the assessment of our model: experimental data can be subject to errors, and the experimental microstructure may deviate from the simulated one. A way to avoid such problems would be to compare our simulations to finite element calculations with similar microstructures. Such data were not available for hypereutectoid steels in the literature. We thus evaluated and selected the considered experimental data with a critical eye, and discussed its quality in the following chapters for [32, 36].

4.5. Virtual microstructural parameter setup

After determining the stiffness matrix and elastic moduli in the modeling, the influence of varied virtual microstructural parameters on the elastic properties of the homogenized macroscopic material was assessed. For this purpose, d_{scem} was chosen among meaningful values, with regards to previous experimental works [37], up to 1 µm. Further, different values of d_{nearl} , λ and ω were assessed, with ω respecting the criteria defined by Eq. (20). We noticed that for both LP/CC and LP/FC, a diversity factor $\Delta = 5$ represented the lower limit to approximate isotropic behavior of the material. Use of a diversity factor $\Delta = 10$ in all calculations, associated with $10^3 = 1000$ different sets of Euler angles, had marginal impact on the calculation time and certified reaching isotropy approximation. All calculations were done on the software MATLAB. Table 2 summarizes the material and microstructural simulation parameters. d_{pearl} and λ were chosen as compromising values between the data given by Elwazri et al. [38] and the constraint of Eq. (20) with a suitable value of ω .

5. Results

The results of our simulations appear to be close to the data found in the literature for μ and E, and the absolute difference between the literature data and our values does not exceed 1.3 GPa (or 1.6% relative difference) for μ and 3.0 GPa (or 1.5% relative difference) for E for all studied microstructures, with a consistently larger difference between the simulation results and the literature data for C_{1111} .

Table 3 compares numerically the simulated values of C_{1111} , C_{1122} and C_{4444} for all modeling cases with experimental data for pearlitic steel from Durgaprasad et al. [36], and

the simulated values of C_{1111} with experimental data of ferritic-pearlitic steel from Kim and Johnson [32]. All simulated terms deviate considerably from the values reported by Durgaprasad et al. [36], whereas the simulated values of C_{1111} match well with the values from Kim and Johnson's work [32]. Note that the term C_{1111} of the stiffness matrix of pearlitic steel obtained by Durgaprasad et al. [36] is lower than C_{1111} of *ferritic*-pearlitic steel as obtained by Kim and Johnson [32] (see Table 2), which clearly justifies the preference of the data from Kim and Johnson for the purpose of simulation validations. Moreover, Kim and Johnson have shown in their work [32] the consistency of their data for ferritic-pearlitic steel with data from several other studies.

Using the same set of material input data, a very small relative difference of less than 0.05% between LP and GP is found for a given θ_s morphology (CC or FC) for the evaluated elastic parameters. For a given pearlite morphology (LP or GP) the relative difference between different θ_s morphologies CC and FC is larger for a particular material input source. It should be noted that the highest values of relative difference between CC and FC (up to 0.20%) are always seen for the simulation of the shear modulus.

In the following, the effects of varied microstructural parameters d_{scem} , d_{pearl} , λ and ω for lamellar pearlitic microstructures LP are assessed, choosing the same material input datasets. We investigate the evolution of the C_{1111} stiffness matrix term, of the shear modulus μ and of the Young's modulus E as a function of d_{scem} and d_{pearl} – see respectively Fig. 2 and Fig. 3 – and compared to the literature references and to the corresponding phase-fraction-weighted averaged moduli.

Simulated C_{1111} (a), μ (b), and E (c) increase slightly with increasing d_{scem} . In contrary, C_{1111} (a), μ (b), and E (c) decrease slightly with increasing pearlite colony size d_{pearl} . The volume-weighted averaged values of C_{1111} , μ and Eshow similar tendencies but less pronounced than for the respective simulated moduli. The larger d_{scem} and the smaller d_{pearl} , the larger the difference between the simulated and averaged values. The influence of varied interlamellar spacing λ or of the lamellae generalized aspect ratio ω on the elastic properties of the homogenized material is not considered here. Despite the relevance of these parameters for industrial applications, to date interrelations between these microstructural features and mechanical properties lie beyond the limitations of the model, which will be discussed in Section 6.2.

For the LP/CC case, we compared our approach using GSCS to the approach using Mori–Tanaka and breaking the rule of separation of scales for different values of d_{scem} and similar input parameters, including the diversity factor Δ . Both methods give similar results for the Young's modulus, see Fig. 4. This result is also discussed in Section 6.2.

6. Discussion

6.1. Trends of evaluated elastic properties

Since material elastic properties differ between α and θ , an increase in the θ phase fraction will shift the values of all elastic parameters of the homogenized material closer to the respective values for pure θ , independent of CC or FC

Table 2. Material and morphological input parameters.

	0	θ (Ledbetter, 2010) [33]							
Phase input data	Bulk modulus (GPa)		Shear modulus (GPa)		Bulk modulus (GPa)		Shear modulus (GPa)		
	167		82		168		90		
Compared elastic steel properties	AISI 1080 steel (Freitas et al., 2010) [35]		Ferritic-pearlitic steel (Kim, Johnson, 2007) [32]		Pearlitic steel (Durgaprasad et al., 2017) [36]				
	Young's modulus (GPa)	Shear modulus (GPa)	<i>C</i> ₁₁₁₁ (GPa)		$C_{1111} = C_{2222} = C_{3333} \text{ (GPa)}$		$C_{1122} = C_{1133} = C_{2233}$ (GPa)		$C_{4444} = C_{5555} = C_{6666} \text{ (GPa)}$
	211.12	81.95	273.9		237		141		116
	Study of the influence of d_{scem}								
Sets of microstruc- tural parameters	$d_{\rm pearl}$ (µm)		$d_{\rm scem}$ (µm)	Interlamellar spacing λ (µm)		Generalized aspect ratio ω		Diversity factor ⊿	
	12		0.1 to 1 (0.1 μm step)	0.14		0.06		10	
	Study of the influence of d_{pearl}								
	$d_{\rm pearl}$ (µm)		$d_{\rm scem}$ (µm)	Interlamellar spacing λ (µm)		Generalized aspect ratio ω		spect	Diversity factor ⊿
	8 to 16 (1 µm step)		0.2	0.14		0.08		10	

characteristics. This behavior is shown in the simulation, testing an increase in d_{scem} , while keeping all other modeling parameters constant, which actually reflects an increase in the θ phase fraction. The bulk and shear moduli of θ according to Ledbetter [33] are higher than the respective data for α taken from Kim and Johnson [32]. Thus, C_{1111} , μ and *E* increase in the simulation with an increasing θ volume fraction. The opposite trend of elastic properties is of course

Table 3. Calculated values of C_{1111} , C_{1122} and C_{4444} for LP or GP and for CC or FC, and absolute and relative difference between the simulated values and the values given by Durgaprasad et al. [36] and by Kim and Johnson for C_{1111} [32].

	C ₁₁₁₁				<i>C</i> ₁₁₂₂			C_{4444}			
Model type	Value (GPa)	Absolute difference (GPa)		Rela diffe: (9	Relative difference (%)		Absolute difference (GPa)	Relative difference (%)	Value (GPa)	Absolute difference (GPa)	Relative difference (%)
		[36]	[32]	[36]	[32]		[36]	[36]		[36]	[36]
LP/CC LP/FC GP/CC	278.01 278.06 278.01	41.01 41.06 41.01	4.11 4.16 4.11	17.30 17.32 17.30	1.50 1.52 1.50	111.72 111.70 111.72	29.28 29.30 29.28	20.77 20.78 20.77	166.29 166.36 166.29	50.29 50.36 50.29	43.35 43.41 43.35
GP/CC	278.01	41.01	4.16	17.30	1.50	111.72	29.28	20.77	166.36	50.36	43.41



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Grain boundary cementite thickness (µm)

(C)

0.8

1.0

θ: [33].

averaged values. Material input data for α : [32]; material input data for

observed in the simulation when d_{pearl} is increased instead of d_{scem} , since an increase in the pearlite colony size means an increase in the volume fraction of pearlite, indirectly associated with a decrease in the volume fraction of θ_{S} . However, the changes in the volume fraction of θ_{S} are only a part of the explanation of the evolution of C_{1111} , μ and E, because the simulated elastic properties would follow their volume-weighted averaged values otherwise. The increasing difference between the simulated and averaged moduli with an increasing θ volume fraction suggests additional microstructural effects, such as an influence of θ_S on the interaction between pearlite colonies for example. Comparison between the present model and finite-element calculation for the same microstructure could provide a more accurate assessment of such effects, besides also improving the demonstration of the calculation quality.

6.2. Limitations of the present model

We noticed no impact of variations of the value of λ or ω on the stiffness matrix C_{mat} of the macroscopic material or C_{ipearl} of the homogenized isotropic pearlite, whereas the stiffness matrix C_{pearl} was affected when only one pearlite colony was considered. Thus, we believe that the constraint of isotropic pearlite, realized by the use of the diversity factor Δ erases the variations in the elastic properties of the pearlite colonies. The use of the Mori–Tanaka method for LP/CC would have the advantage of allowing for contemplation of preferential orientations of pearlite colonies, without mandatory use of Δ . This is relevant for simulations of microstructures with a strong texture, and in the case of plastic deformation. Despite breaking the rule of separation of scales, this approach gave, in fact, similar results to GSCS with the same diversity in orientations of the pearlite colonies. The work of



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Fig. 4. Comparison of the evolution of the simulated Young's modulus as a function of d_{scem} using GSCS (black squares) or using Mori–Tanaka (white dots).

Drugan and Willis [19] on quantitative RVE definitions suggests that ignoring the rule of separation of scales would mostly lead to an increase in local strain variations from the overall strain, decreasing the accuracy of the approximation of elastic moduli used for the definition of an RVE. However, our results suggest that elastic properties of α and θ are sufficiently close to keep local strain variations low. Our work anyway justifies the possibility of further investigations on the effect of texture on the elastic properties of hypereutectoid steels.

The calculated C_{1111} term of the stiffness matrix, the shear modulus μ and the Young's modulus *E* by the present model lie very close to each other for CC and FC morphologies. This implies that the current simplifications of spherical and isotropic pearlite colonies and cementite precipitates cannot reproduce the observation that a decrease in the continuity of the grain boundary θ layer in hypereutectoid steels leads to better mechanical properties [14].

6.3. Outlook

The release of isotropy constraint is necessary in a modification of the generalized self-consistent scheme in order to allow for the conversion of the multiscale mean field homogenization model to a form of texture modeling, which will particularly extend usability towards plasticity modeling. This conforms to the technological fact that microstructural parameters such as λ , d_{scem} , ω , as well as the cementite continuity, are particularly effective beyond the elastic domain [38]. Predictive simulation of this behavior will further have to take into account the effects of the continuity of θ_S on the movement of dislocations within the alloy and on local stress concentrations. Solutions do exist for the construction of Eshelby homogenization methods with non-elliptical inclusions [39]. Such solutions will become particularly relevant in the modeling of microstructures containing Widmanstätten cementite, growing from the grain boundary within the austenite grain as plates or laths [40].

7. Summary and conclusion

We developed four different multiscale mean field calculation schemes for the elastic properties of hypereutectoid steels based on a mean field approach of the Eshelby matrix-inclusion problem in continuum mechanics. These schemes correspond to four types of microstructural interrelations between pearlite and proeutectoid cementite that are typically seen in these alloys. The main input parameters for the modeling are the material input data for cementite and ferrite describing their elastic properties, a set of elastic coefficients such as bulk and shear moduli, or, alternatively, stiffness tensors. A virtual microstructure of hypereutectoid steel consisting of spherical pearlite colonies was constructed by a set of a maximum of four different parameters: 1) the proeutectoid cementite size represented by the thickness of the grain boundary cementite film or the size of individual cementite particles, 2) the size of the pearlite colonies, and in the case of lamellar pearlite, 3) the interlamellar spacing, and 4) the generalized lamellar aspect ratio.

Calculated elastic properties are very close to the experimentally determined values of lamellar pearlitic steels from the literature. These results support the feasibility of the multiscale elasticity homogenization approach for hypereutectoid steel microstructures. For a given set of material input parameters and microstructural parameters, there are only small differences between the results for all evaluated microstructures. These differences are controlled by the thickness of proeutectoid cementite and the pearlite colony size. This result follows the trend of the volume fraction of proeutectoid cementite and pearlite. The diversity of orientations of pearlite colonies in the microstructure probably erases local effects of interlamellar spacing and the generalized aspect ratio of the pearlitic lamellae. Whereas this seems realistic in the elastic domain, a more accurate picture of the influence of the continuous versus fragmented character of proeutectoid cementite on mechanical properties will require the consideration of anisotropy of elastic properties and crystal plasticity in the modeling.

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