Self-consistent one-particle 3D unit cell model for simulation of the effect of graphite aspect ratio on Young’s modulus of cast-iron

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Abstract

The graphite phase of ferritic cast-iron was assumed to consist of randomly oriented, rotationally symmetric, ellipsoidal inclusions of same dimensions. Accordingly, a self-consistent one-particle 3D unit cell model was developed to simulate the effect of graphite aspect ratio on cast-iron elastic constants. The cube shaped unit cell is made up of an inner rotational ellipsoid of graphite surrounded by $\alpha$ Fe–2.5%Si matrix in a concentric outer ellipsoid of the same aspect ratio as the inner graphite ellipsoid in order to model the desired graphite content. The remainder of the unit cell is filled up by the cast-iron compound, the elastic behaviour of which is determined self-consistently. In order to obtain elastic properties, the unit cell was subjected to uniaxial loading. Calculations of stress and strain distributions, in dependence on the orientation of the graphite ellipsoid, were carried out by the finite element method using 3D elements. Finally, updated values of Young's modulus and Poisson's ratio were derived by employing Hooke's law. This procedure was repeated, using the updated elastic constants as new input, to get a self-consistent convergent solution. The results are compared with finite element calculations using a conventional one-particle 3D unit cell model with multiphase elements, and an analytical solution given in the literature. Comparison with experimental data shows the relatively wide range of validity and the superiority of the self-consistent method.

Keywords: Finite element method; Self-consistent unit cell model; Simulation of cast-iron elastic constants

1. Introduction

The subject of this paper is the numerical determination of the elastic behaviour of ferritic cast-iron. An example of a microstructure of ferritic cast-iron is shown in Fig. 1 [1]. It is well known that the shape of graphite particles significantly influences Young’s modulus of cast-iron [2–4]. An analytical formulation of this effect given recently [2,3], Appendix A, is based on a cubic unit cell of $\alpha$ Fe–2.5%Si matrix including a graphite particle of rotational ellipsoidal shape. In a first step, such a unit cell was numerically elaborated in the present work, to recalculate Young's modulus by now employing the finite element method. However, it is evident that the agreement between predicted and experimental Young's modulus is inherently restricted to a limited range of graphite contents and particle aspect ratios. To overcome this difficulty,
in a second step, a more rigorous self-consistent one-particle 3D unit cell method was developed. In this method, the rotational ellipsoidal graphite particle is surrounded by $\alpha$ Fe–2.5%Si matrix forming another larger ellipsoid, both together being embedded in an environment of cast-iron which fills up the cubic unit cell. In this paper, it will be shown that this method yields results in good agreement with the experimental data over a wide range of particle aspect ratios. Furthermore, the method is expected to be applicable to arbitrary graphite contents.

2. First approach: conventional one-particle 3D unit cell model

Fig. 2 shows a schematic of a conventional one-particle 3D unit cell which was used for finite element calculations as a first approach to determine the elastic behaviour of cast-iron. The cubic unit cell was subjected to uniaxial tensile loading along one of the cube edges keeping all the cube faces in plane. Young’s modulus and Poisson’s ratio were determined from the displacements of the cube faces in loading direction, and perpendicular to it. For Poisson’s ratio, the mean displacement along the two cube edges perpendicular to the loading direction was used. The resulting values of Young’s modulus $E(\psi, \varphi)$ and Poisson’s ratio $\nu(\psi, \varphi)$ are dependent on the orientation of the rotational axis of the ellipsoid forming the graphite particle. The average of Young’s modulus and Poisson’s ratio, $E$ and $\nu$, can be calculated as mean values over the orientation of the ellipsoid’s rotational axis which is assumed to be randomly distributed in space:

$$E = \frac{1}{2\pi} \cdot \int_{0}^{\pi/2} \int_{0}^{2\pi} E(\psi, \varphi) \cdot \sin \psi \cdot d\varphi \cdot d\psi$$  \hspace{1cm} (1)
$$\nu = \frac{1}{2\pi} \cdot \int_{0}^{\pi/2} \int_{0}^{2\pi} \nu(\psi, \varphi) \cdot \sin \psi \cdot d\varphi \cdot d\psi$$  \hspace{1cm} (2)

The angles $\psi$ and $\varphi$ define the spatial position of the ellipsoid: The ellipsoid’s rotational symmetry axis is inclined to the load line by $\psi$, and rotated about it by $\varphi$. Eqs. (1) and (2) are approximated replacing the integration of $E(\psi, \varphi)$ over $\varphi$ by simply averaging the values for $\varphi = 0$ (ellipsoid’s rotational axis in a plane parallel to a cube face) and $\varphi = \pi/4$ (ellipsoid’s rotational axis in a cube’s diagonal plane), and approximating further integration over $\psi$ by Kepler’s rule:

$$E = \frac{\pi}{12} \cdot \left[ 2 \cdot \sqrt{2} \cdot \frac{E(\pi/4, 0) + E(\pi/4, \pi/4)}{2} + \frac{E(\pi/2, 0) + E(\pi/2, \pi/4)}{2} \right]$$  \hspace{1cm} (3)

$$\nu = \frac{\pi}{12} \cdot \left[ 2 \cdot \sqrt{2} \cdot \frac{\nu(\pi/4, 0) + \nu(\pi/4, \pi/4)}{2} + \frac{\nu(\pi/2, 0) + \nu(\pi/2, \pi/4)}{2} \right]$$  \hspace{1cm} (4)
Finite element calculations were carried out using multiphase elements, i.e. the meshes are fixed for different positions of the ellipsoid ($\psi$ and $\varphi$) such that elements at the interface of the matrix and the graphite can possess integration points within either of the two phases.

3. Second approach: self-consistent one-particle 3D unit cell model

The self-consistent one-particle 3D unit cell model is schematically illustrated in Figs. 3 and 4. The unit cell is again a cube, however, in this case it is subdivided into three phases, i.e. graphite, $\alpha$ Fe–2.5%Si matrix and cast-iron, Fig. 3. The matrix fills the space between the inner ellipsoid (graphite) and an outer larger ellipsoid with the same aspect ratio. In this way the model will in principle not be restricted in the choice of the aspect ratio. The embedding cast-iron serves as a realistic boundary condition and, therefore, must be of sufficient extent. For the present calculations, the edge length of the cube was taken to be five times that of the longer axis of the outer ellipsoid. The unit cell was again subjected to uniaxial tensile loading along one of the cube axes ($y$-direction), and the cube faces were kept in plane. The spatial orientation of the ellipsoids is shown in Fig. 4, and corresponds to the description given in Section 2.

In a first step, the volumetric mean stress tensor $\bar{\sigma}(\psi, \varphi)$ and the volumetric mean total strain tensor $\bar{\varepsilon}(\psi, \varphi)$ were calculated over the volume $V$ of the outer ellipsoid (including the inner ellipsoid), i.e. the $\alpha$ Fe–2.5%Si matrix and the graphite, as a function of the orientation angles $\psi$ and $\varphi$ (Fig. 4):

$$\bar{\sigma}(\psi, \varphi) = \frac{1}{V} \cdot \int_{V} \bar{\sigma}(x,y,z) \cdot dV$$

$$\bar{\varepsilon}(\psi, \varphi) = \frac{1}{V} \cdot \int_{V} \bar{\varepsilon}(x,y,z) \cdot dV$$

Here, $x, y, z$ denote the spatial coordinates in the global coordinate system with axes given by 1, 2, 3. In terms of finite elements this can be written as

$$\bar{\sigma}(\psi, \varphi) = \frac{\sum_{k} \bar{\sigma}_{k} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}}$$

$$\bar{\varepsilon}(\psi, \varphi) = \frac{\sum_{k} \bar{\varepsilon}_{k} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}}$$

where $k$ is the index of summation over all integration points located within the outer ellipsoid, and $\Delta V_{k}$ are the corresponding volumes allocated to these integration points by the finite element code. These calculations were carried out in an especially developed user defined subroutine.
In the next step, the tensors \( \bar{\sigma}(\psi, \varphi) \) and \( \bar{\varepsilon}(\psi, \varphi) \) obtained from the finite element simulations were averaged with respect to \( \psi \) and \( \varphi \) by a post-processing procedure, presuming a random spatial distribution of the orientation of the graphite ellipsoid’s rotational symmetry axis:

\[
\bar{\sigma} = \frac{1}{2\pi} \int_{0}^{\pi/2} \int_{0}^{2\pi} \bar{\sigma}(\psi, \varphi) \cdot \sin \psi \cdot d\varphi \cdot d\psi
\]

\[
\bar{\varepsilon} = \frac{1}{2\pi} \int_{0}^{\pi/2} \int_{0}^{2\pi} \bar{\varepsilon}(\psi, \varphi) \cdot \sin \psi \cdot d\varphi \cdot d\psi
\]  

(9)

As the cast-iron matrix around the outer ellipsoid is sufficiently large, it can be approximately assumed that the tensors \( \bar{\sigma}(\psi, \varphi) \) and \( \bar{\varepsilon}(\psi, \varphi) \) exhibit rotational symmetry. This means that the elements of the tensors \( \bar{\sigma}(\psi, \varphi) \) and \( \bar{\varepsilon}(\psi, \varphi) \) in the coordinate system rotated by \( \varphi \) are virtually identical to the elements of the tensors \( \bar{\sigma}(\psi, 0) \) and \( \bar{\varepsilon}(\psi, 0) \), respectively, in the reference coordinate system defined by \( \varphi = 0 \). The angle \( \varphi = 0 \) means the reference position which is arbitrarily chosen by positioning the graphite ellipsoid’s symmetry axis parallel to a cube face. Therefore, a finite element calculation is needed for \( \varphi = 0 \) only. The integration over \( \varphi \) in Eqs. (9) and (10) yields, after transformation of \( \bar{\sigma}(\psi, \varphi) \) and \( \bar{\varepsilon}(\psi, \varphi) \) to the reference coordinate system, the elements of the mean tensors \( \bar{\sigma} \) and \( \bar{\varepsilon} \) as:

\[
\sigma_{11} = \sigma_{33} = \int_{0}^{\pi/2} \frac{1}{2} \cdot [\sigma_{11}(\psi, 0) + \sigma_{33}(\psi, 0)] \cdot \sin \psi \cdot d\psi
\]

\[
\sigma_{22} = \int_{0}^{\pi/2} \sigma_{22}(\psi, 0) \cdot \sin \psi \cdot d\psi
\]

(11)

(12)

\[
\sigma_{12} = \sigma_{13} = \sigma_{23} = 0
\]

(13)

\[
\varepsilon_{11} = \varepsilon_{33} = \int_{0}^{\pi/2} \frac{1}{2} \cdot [\varepsilon_{11}(\psi, 0) + \varepsilon_{33}(\psi, 0)] \cdot \sin \psi \cdot d\psi
\]

\[
\varepsilon_{22} = \int_{0}^{\pi/2} \varepsilon_{22}(\psi, 0) \cdot \sin \psi \cdot d\psi
\]

(14)

(15)

\[
\varepsilon_{12} = \varepsilon_{13} = \varepsilon_{23} = 0
\]

(16)

The integrations in Eqs. (11)–(16) were carried out by Simpson’s rule subdividing the integration interval \((0, \pi/2)\) into six equal parts, i.e. according to six equidistant positions of \( \psi (\pi/12 \text{ to } \pi/2) \). The resulting elements \( \sigma_{ij} \) and \( \varepsilon_{ij} \) of the mean tensors \( \bar{\sigma} \) and \( \bar{\varepsilon} \) of Eqs. (9) and (10) were then used to calculate the next approximation of Young’s modulus and Poisson’s ratio of cast-iron using Hooke’s law.

The whole procedure was repeated (three times), using updated values of \( E \) and \( \nu \) in order to achieve convergence. As a starting point, \( E \) and \( \nu \) of cast-iron were initially set to the values of the \( \alpha \) Fe–2.5%Si matrix.

In case of spherical graphite particles, an axisymmetric calculation can be carried out, and the angles \( \psi \) and \( \varphi \) are meaningless. When using axisymmetric finite elements, Eqs. (7)–(16) have to be replaced by:

\[
\sigma_{11} = \sigma_{33} = \frac{1}{2} \cdot \left\{ \frac{\sum_{k} \sigma_{11}^{(k)} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}} + \frac{\sum_{k} \sigma_{33}^{(k)} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}} \right\}
\]

(17)

\[
\sigma_{22} = \frac{\sum_{k} \sigma_{22}^{(k)} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}}
\]

(18)

\[
\sigma_{12} = 0
\]

(19)

\[
\varepsilon_{11} = \varepsilon_{33} = \frac{1}{2} \cdot \left\{ \frac{\sum_{k} \varepsilon_{11}^{(k)} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}} + \frac{\sum_{k} \varepsilon_{33}^{(k)} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}} \right\}
\]

(20)

\[
\varepsilon_{22} = \frac{\sum_{k} \varepsilon_{22}^{(k)} \cdot \Delta V_{k}}{\sum_{k} \Delta V_{k}}
\]

(21)

and

\[
\varepsilon_{12} = 0
\]

(22)

The index \( k \) again denotes the integration point number. The tensor elements \( \sigma_{13}, \sigma_{23}, \varepsilon_{13}, \varepsilon_{23} \) are trivially zero because of axisymmetry. It should be noted that, in this case (axisymmetry), \( \Delta V_{k} \) means a ring-shaped volume element, and the integration over the volume takes into account the rotation of the coordinate system about the \( y \)-axis (axis no. 2).
Eqs. (17)–(22) are obtained by averaging with respect to rotation of the coordinate system about the symmetry axis (y-direction).

4. Determination of aspect ratio from metallographic observations

In the present paper, the data on elastic properties of cast-iron by Lõhe et al. [4] are used. In order to determine the aspect ratio \( c/a \) of the ellipsoidal inclusion, it is necessary to convert Lõhe’s parameter \( \eta \):

\[
\eta = \text{Average of } \left( \frac{\pi}{4} \frac{S_{\text{max}}^2}{\text{area}} \right)
\]

where \( S_{\text{max}} \) is the maximum intercept size of a particle, ‘area’ means the sectional area of this particle in an arbitrarily chosen cross-sectional (metallographic) plane, and the average is carried out over the particles observed in the metallographic section. Assuming the particles can be approached by rotational ellipsoids of the same shape and size, they will appear in the cross-sectional plane as ellipses of various shapes and sizes.

The parameter \( \eta \) is then defined by the ratio of the longer semi-axis length \( C \) and the shorter semi-axis length \( A \) of these ellipses averaged over the particles in the cross-sectional plane:

\[
\eta = \text{Average of } \left( \frac{C}{A} \right)
\]

The elliptical axis ratio \( C/A \) can be calculated from graphite ellipsoid’s aspect ratio \( c/a \), Fig. 4, intersecting the graphite ellipsoid by the cross-sectional plane, and employing analytical geometry [5]:

\[
\left( \frac{C}{A} \right) = \frac{\sin^2 \vartheta + (c/a)^2 \cdot \cos^2 \vartheta}{c/a} \quad \text{for } c/a < 1
\]

\[
\left( \frac{C}{A} \right) = \frac{c/a}{\sin^2 \vartheta + (c/a)^2 \cdot \cos^2 \vartheta} \quad \text{for } c/a > 1
\]

Here, \( \vartheta \) means the angle between the cross-sectional plane normal and the rotational symmetry axis of the graphite ellipsoid.

The distribution function of the orientation angles \( \vartheta \) of those graphite ellipsoids intersected by the cross-sectional plane, assuming their random orientation in space, is given by [5]

\[
P(\vartheta) = \frac{\sqrt{\sin^2 \vartheta + (c/a)^2 \cdot \cos^2 \vartheta \cdot \sin \vartheta}}{\int_0^{\pi/2} \sqrt{\sin^2 \vartheta + (c/a)^2 \cdot \cos^2 \vartheta \cdot \sin \vartheta} \cdot d\vartheta}
\]

Eq. (27) was derived from the requirement that \( P(\vartheta) \) should be proportional to the distance \( 2\sqrt{a^2 \sin^2 \vartheta + c^2 \cos^2 \vartheta} \) of the two planes parallel to the cross-sectional plane being tangential to the graphite ellipsoid, and also proportional to the overall distribution function of the angles \( \vartheta \) in space, i.e. \( \sin \vartheta \) for random distribution.

Lõhe’s parameter \( \eta \) is then given by [5]:

\[
\eta = \int_0^{\pi/2} \left( \frac{C}{A} \right) \cdot P(\vartheta) \cdot d\vartheta
\]

where \( C/A \) is derived from Eqs. (25) and (26) as a function of \( \vartheta \).

The integration can be carried out in closed form, and the final result is [5]:

\[
\eta = \frac{2 + (c/a)^2}{3 \cdot (c/a)^2} \left( 1 + \frac{2}{\arccos(c/a)} \right) \quad \text{for } c/a < 1
\]

\[
\eta = \frac{2 \cdot (c/a) \cdot \sqrt{(c/a)^2 - 1}}{(c/a) \cdot \sqrt{(c/a)^2 - 1} + \ln \left( \frac{(c/a) + \sqrt{(c/a)^2 - 1}}{1}\right)} \quad \text{for } c/a > 1
\]

The case \( c/a = 1 \) is trivial and yields \( \eta = 1 \).

Fig. 5 shows a plot of \( \log_{10} \eta \) versus \( \log_{10} (c/a) \). It can be seen that, for sufficiently small aspect ratios \( c/a < 1 \) (discs), any value of \( \eta \) can be reached; for \( c/a > 1 \) (needles), however, \( \eta \) is limited to \( \eta \leq 2 \) (\( \eta \rightarrow 2 \) for \( c/a \rightarrow \infty \), Eq. (30)). This means that in case \( \eta \) is experimentally determined to be less than 2, two interpretations for the shape of the graphite inclusions, disc or needle, are possible. In the case of \( \eta > 2 \) the graphite ellipsoid...
under the assumption of rotational symmetric particles can only be interpreted to be of disc shape.

5. Experimental database and theoretical results

The experimental data on elastic properties were taken from Löhe et al. [4]. They are listed in Table 1 along with the values of \( c/a \) determined by using Eqs. (29) and (30). It is shown that the interpretation \( c/a > 1 \) is only possible in cases where the graphite particle shape is near spherical. However, there is one specimen (GGV) with \( \eta > 2 \), i.e. \( c/a \) should be less than 1, which nevertheless was judged by Löhe et al. [4] to display needle-like graphite particles. This judgement was based on SEM examination on a cross-section which was heavily etched in order to reveal the 3D shape of near surface particles. However, the present theory suggests that the interpretation “needle-like rotational ellipsoid” is not acceptable in this case, and in fact the original SEM micrograph of specimen GGV [4] rather displays a linked vermicular microstructure.

The finite element calculations were carried out using the finite element code ABAQUS [6]. The results of the two approaches (Sections 2 and 3) are given in Tables 2 and 3. The graphite volume fraction \( V_G \) was set to 0.10 and 0.12 since all the experimental values (Table 1) are within this range. The first approach (conventional unit cell model) is restricted to \( c/a > 6/\pi \cdot V_G \ (c/a < 1) \) or \( c/a < \sqrt{\pi/(6 \cdot V_G)} \ (c/a > 1) \), since the graphite particle must not penetrate the cube faces of the unit cell. In contrast, the second approach (self-consistent unit cell model) could be used over a wide range of \( c/a \) values. The calculations with both models were carried out setting the elastic properties of the \( \alpha \) Fe–2.5%Si matrix to \( E_M = 206000 \) MPa, \( \nu_M = 0.290 \) [4], and of the graphite inclusions to \( E_G = 4170 \) MPa, \( \nu_G = 0.2225 \) [4, 7]. In Fig. 6, the results of these calculations are shown.

![Graph](image)

**Fig. 5.** Conversion of Löhe's parameter \( \eta \) to the aspect ratio \( c/a \) of rotational symmetric ellipsoidal particles. Definition: \( \eta = \) average value of \( \pi/4 \cdot S_{\text{max}}/\text{area} \) \((S_{\text{max}} = \text{maximum intercept size of particle}, \ \text{‘area’} = \text{sectional area of particle})\) [4].

<table>
<thead>
<tr>
<th>Specimen</th>
<th>Graphite particle shape by SEM</th>
<th>Graphite content [vol. %]</th>
<th>Löhe’s parameter ( \eta )</th>
<th>Ellipsoidal aspect ratio ( c/a ) (determined from ( \eta ))</th>
<th>Young’s modulus [GPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>GGG-A</td>
<td>Sphere(^a)</td>
<td>11.3</td>
<td>1.31</td>
<td>0.698</td>
<td>171</td>
</tr>
<tr>
<td>GGG-B</td>
<td>Sphere(^a)</td>
<td>11.5</td>
<td>1.62</td>
<td>0.546</td>
<td>172</td>
</tr>
<tr>
<td>GGG-C</td>
<td>Sphere(^a)</td>
<td>11.3</td>
<td>1.55</td>
<td>0.574</td>
<td>170</td>
</tr>
<tr>
<td>GGG-D</td>
<td>Sphere(^a)</td>
<td>11.8</td>
<td>1.34</td>
<td>0.679</td>
<td>169</td>
</tr>
<tr>
<td>GGV</td>
<td>Needle</td>
<td>11.3</td>
<td>2.91</td>
<td>0.294</td>
<td>–</td>
</tr>
<tr>
<td>GG-A (1)</td>
<td>Disc</td>
<td>11.5</td>
<td>32.6</td>
<td>0.0261</td>
<td>83</td>
</tr>
<tr>
<td>GG-A (2)</td>
<td>Disc</td>
<td>11.5</td>
<td>37.3</td>
<td>0.0228</td>
<td>81</td>
</tr>
<tr>
<td>GG-A (3)</td>
<td>Disc</td>
<td>11.5</td>
<td>38.9</td>
<td>0.0218</td>
<td>79</td>
</tr>
<tr>
<td>GG-A (4)</td>
<td>Disc</td>
<td>11.5</td>
<td>40.7</td>
<td>0.0208</td>
<td>76</td>
</tr>
<tr>
<td>GG-B</td>
<td>Disc</td>
<td>11.3</td>
<td>26.7</td>
<td>0.0318</td>
<td>88</td>
</tr>
<tr>
<td>GG-C</td>
<td>Disc/needle</td>
<td>10.9</td>
<td>6.41</td>
<td>0.132</td>
<td>135</td>
</tr>
</tbody>
</table>

\(^a\) Near spherical.
and compared to the analytical solution by Boc-
caccini [2], and the experimental data by L€

oohe et al. [4]. It can be seen that the results of both finite
element models satisfactorily match the experi-
mental data, although the self-consistent unit cell
method is superior because of its wider range of
application. The performance of the analytical
method, however, is relatively poor, and it fails in
the regime of very flat discs (c/a < 0.1). It should
be noted that even Young’s modulus of specimen
GGV is met by the self-consistent unit cell method
when interpreting the graphite particles as disc
shaped according to Section 4.

6. Discussion and conclusions

The self-consistent one-particle 3D unit cell
model turned out to be very useful in predicting
the elastic properties of cast-iron as a function of
the graphite particle shape. The assumption of
rotational symmetric ellipsoidal particles and the
assumption of isotropic elastic behaviour of
graphite obviously is a sufficiently good approach
to the elastic properties of cast-iron. For the sake
of completeness, ellipsoids with aspect ratios
c/a < 1 (discs) and c/a > 1 (needles) have both
been examined. However, the assumption of as-
pect ratios c/a > 1 was not very efficient: Either it
was not possible to interpret, based on average η
values (Eq. (23)), the actual graphite inclusions as
 ellipsoids with aspect ratios c/a > 1 (for η ≥ 2,
Fig. 5), or the particle shape was too close to a
sphere (Fig. 6) for the c/a ratio to have an effect on
the elastic constants. Thus, further consideration
of aspect ratios c/a > 1 is not necessary in the
present context, although it may be important in
case of other compound materials.

The self-consistent method is in principle not
restricted in the choice of the aspect ratio of the
graphite inclusions. Even for a small aspect ratio
of c/a = 1/20 it worked satisfactorily well. The
model also fulfills the limiting condition that for
a graphite volume fraction approaching 1, the
properties of graphite will be reached. Moreover,
as it is a one-particle theory, the computing times will also allow for modeling of the plastic and even viscoplastic or creep properties. The next step will be the prediction of plastic behaviour of cast-iron.

Recently, a finite element method using a multi-particle 3D unit cell was presented [8]. The particle shape was again approached by rotational symmetric ellipsoids. This model was successfully applied to predict the elastic behaviour of Al/SiC composites. It would be interesting to use this model also for cast-iron, and to compare the results with those achieved by the self-consistent one-particle unit cell model developed in the present paper. Although the multi-particle unit cell model is, in principle, certainly more realistic, it obviously takes much more finite elements and hence longer computing times. This may give rise to restrictions in case of more time-consuming material descriptions, e.g. visco-plasticity.

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Appendix A

An analytical formula for the effective Young’s modulus $E$ of a composite made of ferritic matrix and graphite inclusions is given by Boccaccini [2]:

$$E = E_M \left\{ 1 - \frac{\pi}{A} \left[ 1 - \frac{1}{9 \left( 1 + \frac{1.99}{B} \left\{ \frac{E_M}{E_G} - 1 \right\} \right)} \right] \right. $$

$$\left. \left( 1 + \frac{1.68}{B} \left\{ \frac{E_M}{E_G} - 1 \right\} \right) \right\} - \frac{5}{9 \left( 1 + \frac{1.04}{B} \left\{ \frac{E_M}{E_G} - 1 \right\} \right)} \right\}$$

with

$$A = \frac{\left( \frac{4\pi}{3V_G} \right)^{2/3} \left( \frac{c}{a} \right)^{-1/3}}{\sqrt{1 + \left( \left[ \frac{c}{a} \right]^2 - 1 \right) \cos^2 \psi}}$$

and

$$B = \left( \frac{4\pi}{3V_G} \right)^{1/3} \left( \frac{c}{a} \right)^{1/3} \sqrt{1 + \left( \left[ \frac{c}{a} \right]^2 - 1 \right) \cos^2 \psi}$$

where $E_M$ and $E_G$ are Young’s moduli of the ferritic matrix and the graphite inclusions, respectively, and $V_G$ is the volume fraction of the inclusions. $c/a$ denotes the aspect ratio of the ellipsoidal inclusions, and $\psi$ is the angle between the rotational axis of the ellipsoid and the load direction (Fig. 4). Setting $\cos^2 \psi = 0.33$ gives an average value of $E$ for a random statistical orientation of the ellipsoids [2].

It should be noted that, according to Boccaccini [9], there is a typographical error in the original formula [2] for $B$ above, where, in the original paper, the exponent of $c/a$ under the square root is erroneously 2 instead of $-2$.

In [2], $E_G$ was set to be 8500 MPa instead of 4170 MPa (lower third-order-bound [7]) used for the present calculations. However, this assumption makes only a minor difference, and does not have any influence on the conclusions drawn in the present publication.

References


