Plastic deformation behaviour of Fe–Cu composites predicted by 3D finite element simulations

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A B S T R A C T
Two-phase composites, which consist of polycrystalline α-iron and copper particles, are studied mechanically under large plastic deformation. Due to the significant difference of the yield stress in the iron and the copper phase in which the slip system geometry is also dissimilar, a high heterogeneity and anisotropy characterize the plastic deformation behaviour. In this work, an elastoviscoplastic material model is applied in finite element simulations, whereas the macroscopic material behaviour is established based on constitutive equations of the single crystal. Due to the natural spatial character of the slip system mechanisms of crystal plasticity, the numerical calculation must be performed fully 3D. However, since it is hardly possible to determine the grain geometry of a real material in 3D without destroying the sample by slicing or the like, real 2D cross-sections have been modelled and extended to the third dimension in an axisymmetric way producing an annular pattern, which comes closer to reality than a 2D structure. Numerical predictions include the grain deformation behaviour, the flow behaviour, the crystallographic texture, and the local strain in Fe–Cu composites. In particular, a quantitative study is performed for the mean value of the local strain in both phases, which shows a good agreement with the experimental result for the Fe17–Cu83 composite under tension.

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1. Introduction

Multiphase metals are widely applicable in the automobile and aerospace industries, since they can show good ductility, enhanced strength at elevated temperature, and improved corrosion resistance. During the deformation process in such polycrystals, the microstructure and its evolution are essential for the determination of the macroscopic mechanical behaviour. The main features of the microstructure include the morphology, the arrangement, and the orientation of grains. The volume fraction of each phase and the interaction among grains are also important factors which influence the macroscopic material properties.

To investigate the influence of local mechanical interactions among the phases on the plastic behaviour in such polycrystals, α-Fe–Cu composites as model materials have been studied in this work. The iron and the copper phase have significantly different strengths, dissimilar crystal structures, simple slip geometries, and negligible solubility into each other [5]. Furthermore, the mechanical behaviour of these single phase materials (pure iron and pure copper) are relatively well understood. Commentz et al. [6], Commentz [5], Hartig and Mecking [8] and Daymond et al. [7] investigated for the first time the complex plastic deformation of this type of composite. Here, we introduce a mechanical approach [16] based on finite elements to numerically study properties of iron–copper composites and compare the results with experimental data [5]. Because of the geometry of the slip system mechanisms of crystal plasticity, the numerical calculation must be fully three-dimensional (3D). The interaction between grains and phases is important for the deformation process in two-phase polycrystals [17]. Therefore, the cutouts of real microstructures of the Fe17–Cu83 and the Fe50–Cu50 composite are used as the cross-sections and have been extended in the third dimension in an axisymmetric way, in which regions near the grain boundaries are finer meshed than other parts. To achieve reasonable computing time, we incorporate realistic two-dimensional (2D) morphologies, the internal interphase, and the crystallographic texture in these calculations to predict the micro and macromechanical properties of Fe–Cu composites under simple tensile and compressive loads until large plastic strains.

This work is structured as following. The production of samples and processes of experimental tests are briefly introduced in...
Section 2. In Section 3, we summarize the constitutive equations for single crystals. The material behaviour of polycrystals is established based on the above mentioned equations of the single crystal. Section 4 introduces the finite element model applied in this work. Section 5 indicates the numerical predictions, which concern local and global deformation properties of Fe–Cu composites, and are compared with experimental results. Firstly, we present the local deformation behaviour of grains. The flow behaviour is not only characterized by stress–strain curves but also discussed by the stress evolution in each phase according to the orientation distribution of the grains and the increasing plastic deformation. The crystallographic texture of the composites is presented by standard inverse pole figures for each phase, and a comparison between the prediction and the experimental measurement is given. The numerical and experimental data of the strain distribution is presented for the Fe17–Cu83 composite at about 20% plastic strain.

Notation. In the present work, 2nd- and 4th-order tensors are presented as \( A \) and \( A^\top \), respectively. \( A^{-1} \), \( A^\top \) and \( A \) indicate the inverse, the transpose and the material time derivative of the tensor \( A \). The mapping of a 2nd-order tensor and a 4th-order tensor is presented as \( A/B \). \( ||A|| \) denotes the norm of tensor \( A \).

2. Experiment

Iron-copper composites are produced from mixtures of iron and copper powders by powder metallurgy. Such powders have a purity higher than 99.9% and consist of spherical polycrystalline particles with a diameter less than 63 \( \mu \text{m} \). The mean value of the particle size is 20.5 \( \mu \text{m} \) for the iron phase and 18.3 \( \mu \text{m} \) for the copper phase. Such a production of iron–copper polycrystals follows three steps: the mixing, the precompression, and the final compression. The porosity of the composite is <1 vol.%, and the samples are named in the volume fraction after the composition. Fig. 1 shows the microstructure of the aforementioned Fe–Cu polycrystals (after composition) where the darker phase represents the iron.

The stress–strain behavior is studied by compressive tests which are performed on cylindrical samples (height: 9 mm, diameter: 6 mm) at room temperature with a constant strain rate \( \dot{\varepsilon} = 10^{-4} \text{ s}^{-1} \). The experiments have been performed by Commentz et al. [6]. The detailed information concerning the experiment can be found in Commentz et al. [6] and Commentz [5]. The \( \sigma – \varepsilon \) curves are friction corrected with a friction coefficient \( \mu = 0.235 \). After the compression test (90% logarithmic plastic strain), the sample is ground and polished until its middle plane being parallel to the top and bottom surface is laid open. The texture measurement is accomplished on this middle surface. Pole figures are measured for three reflections, namely \{200\}, \{211\} and \{220\} for the iron phase and \{200\} \{220\} \{311\} for the copper phase, by scanning the hexagonal grid [13]. The measured data are further processed in a 5 \( \times \) 5 grid.

The local resolved strain is performed on a tension sample of the Fe17–Cu83 composite. The measured cutout is extracted from the middle plane (through the tension direction and the transverse direction) of the unloaded sample, and has a rectangular geometry with a dimension of 640 \( \times \) 480 \( \mu \text{m}^2 \) and 160 \( \times \) 120 \( \mu \text{m}^2 \) for the undeformed case and at large deformations, respectively. The grid of sampling points is 3 \( \times \) 3.

3. Crystal plasticity modelling

3.1. Elastic law

We denote the deformation gradient by \( F \) and the plastic transformation by \( P \) [2,3].

\[
F := FP.
\]

This leads formally to the same decomposition suggested, e.g., by Lee (1969), if we identify \( F_P \) by \( P^{-1} \), i.e., \( F = F_P F_p \). \( F_p \) indicates the elastic distortion, the dilatation and the rotations which also account for rigid body rotations. \( F_R \) consists of crystallographic slips along the slip systems \((d_s, n^s)\). The plastic incompressibility implies \( \det (F_P) = 1 \).

Since the elastic strains in our materials are small, we assume a linear relation between the 2nd Piola–Kirchhoff stress \( S_p = \det^{-1}(F_P)F_{P}^{-1} aF_{p}^{-T} \) with the Cauchy stress \( \sigma \) and Green’s strain \( E_s^C \) in the undistorted configuration

\[
S_p = \tilde{c} E_s^C, \quad E_s^C = \frac{1}{2}(C_s - I),
\]

with \( \tilde{c} \) (constant) elasticity tensor \( \tilde{c} \), the elastic right Cauchy–Green tensor \( C_s = F_P^{-1} F_{p}^{-1} \), and the 2nd-order unit tensor \( I \). A tilde indicates that a quantity is formulated with respect to the undistorted configuration which is characterized by the fact that corresponding symmetry transformations are elements of \( SO(3) \). The Kirchhoff stress tensor \( \sigma^R \) is given by \( \sigma^R = F_P S_p F_P^{-T} \).

3.2. Flow rule

The flow rule is taken from finite crystal visco-plasticity theory which specifies the time evolution of \( P \) in terms of the shear rate \( \dot{\gamma}_s \) and the Schmid tensors \( \mathbf{M}^s \) (\( s = 1 \ldots N \), with \( N \) the number of slip systems). The shear rates \( \dot{\gamma}_s \), the Schmid resolved shear stresses \( \tau_s \), and the Schmid tensors \( \mathbf{M}^s \) are given as

![Table of Fe–Cu polycrystals with the different phase volume fraction](image)

Fig. 1. Microstructures of Fe–Cu polycrystals with the different phase volume fraction [5].

\footnote{In this work, \( \varepsilon \) and \( \varepsilon_p \) present the true total strain and the plastic strain in a given direction, respectively.}
\[ \dot{\gamma}_2 = \dot{\gamma}_0 \text{sgn}(\tau_a) \left| \frac{\tau_a}{\tau_0} \right|^m, \]
\[ \tau_x = C_SM_x \approx S_x \cdot M^x, \]
\[ M^x = \hat{d}_x \otimes \hat{n}_x, \]

respectively [9]. The constant \( \dot{\gamma}_0 \) is called reference shear rate and \( m \) is the strain rate sensitivity parameter. A certain slip system \( x \) is specified by the slip direction \( \hat{d}_x \) and the slip plane normal \( \hat{n}_x \). For a given \( L = F F^{-1} \), the flow rule can be formulated in terms of \( F \),
\[ \dot{F}_t F^{-1} = L - F \dot{k}(T_c, \tau_c) F_t, \]
\[ \dot{k}(T_c, \tau_c) = \sum_{i=1}^{N} \gamma_i(T_c, \tau_c) M^i, \]

where \( T_c = F_t^T F F_t \) is the Mandel tensor. For \( F(0) = I \), the initial condition of the differential Eq. (4) is given as \( F(0) = Q_0 \in SO(3) \), where \( Q_0 = g_0(0) \otimes e \) is the initial orientation of the single crystal with the lattice vectors \( g_0 \) and the orthonormal basis \( e \). It is a reasonable assumption that the slip systems of fcc materials harden isotropically [11] such that only one critical resolved shear stress \( \tau_c \) appears in Eq. (4). For simplicity and limited by the experimental data, this concept is also applied to the iron phase of the Fe–Cu composites. Slip systems of copper and iron are chosen as \{110\} \{111\} and \{111\} \{110\} [8], respectively.

3.3. Hardening rule

The materials under consideration have been submitted to monotonous deformations (simple tension and compression) at room temperature. Under such conditions, the plastic deformation is characterized by the accumulation of dislocations in the crystal lattice. The Kocks–Mecking hardening rule, which emphasizes the mechanisms of the dislocation growth, the accumulation, and the annealing is a suitable rule to be applied for materials in this work. It is applicable for both fcc and bcc crystals to predict the material behaviour, accordingly [11].

The critical resolved shear stress \( \tau_c \) can be related to the mean dislocation density \( \rho \) in the form
\[ \tau_c = 2 b \mu \sqrt{\rho}, \]
with the shear modulus \( \mu \), \( b \) in Eq. (5) denotes the magnitude of the Burgers vector. The scalar \( \alpha \) depends weakly on the temperature and the strain rate. Here, it is considered as constant. In the context of the finite deformations, the evolution of \( \rho \) can be given as
\[ \hat{\rho}(\tau_x, \rho) = \left( \frac{\sqrt{\rho}}{b \mu} - \kappa \right) \left| \frac{\rho}{\rho_0} \right|^{1/4} \dot{\gamma}(\tau_x, \rho), \]
\[ \dot{\gamma} \text{ in Eq. (6) is expressed as} \]
\[ \dot{\gamma}(\tau_x, \rho) = \sum_{i=1}^{N} \left| \dot{\gamma}_i(\tau_x, \tau^c(\rho)) \right|. \]

In Eq. (6), \( n \) denotes the stress exponent and \( \frac{\rho_0}{\rho} \) is a material constant (10^7 s^-1). Other values of \( \frac{\rho_0}{\rho} \) are possible for different materials, but it should be based on the values from experiments and kept in agreement with the order of magnitude expected from the dislocation theory [11]. \( \kappa \) is a factor related to the temperature, and \( \beta \) denotes the proportionality constant for the slip system density \( \rho \) and the average slip distance. \( N \) in Eq. (7) is the number of slip systems. Detailed information as to work-hardening can be found in Kocks [10] and Kocks and Mecking [11]. The hardening rule is presented by
\[ \tau^c = \Theta_0 \left( 1 - \frac{\tau^c(\tau_x, \tau^c)}{\tau_c(\tau_x, \tau^c)} \right) \dot{\gamma}(\tau_x, \tau^c), \]

where
\[ \tau_c = \frac{\tau_{c}^0}{\tau_0} \left| \frac{\tau_a}{\tau_0} \right|^m. \]
\[ \Theta_0 = \frac{\tau_{c}^0}{\tau_0} \text{ and } \tau_{c}^0 = \frac{\tau_{c}^0}{\tau_0} \text{ are input material parameters which can be identified from experiments. The reference shear rate } \dot{\gamma}_0 \text{ is a constant.} \]

3.4. Homogenization of stresses

The above constitutive equations are suitable for a single crystal. Materials in this work are assumed to be free of pores and cracks. To describe the transition from the micro to the macro variables, we apply the representative volume element (RVE). Macro fields are determined through homogenising the corresponding micro fields by appropriate averages over the RVE. The effective Kirchhoff stress tensor is given by the volume average over the reference volume \( V \)
\[ \varepsilon = \frac{1}{V} \int_V \varepsilon dV. \]

4. Finite element simulation

4.1. Identification of the morphology and meshing technique

To predict the deformation behaviour of Fe–Cu polycrystals, an axisymmetric model is used in the finite element simulation which is well applicable for complex structures, inhomogeneities, and anisotropies. The axisymmetric simulation\(^2\) with the assumption of a finite length in the third direction (hoop direction) should give better predictions than 2D ones with the assumption of the infinite length in the third direction. Here, the cross-sections of axisymmetric models are identified from the cutouts of real microstructures. In order to emphasize the interaction among the grains, the regions near the grain boundaries are finer meshed than other parts. Such a mesh can be generated by the public domain software OOF [14]. The numerical simulations are performed by ABAQUS [11].

Figs. 2 and 3 with subfigures a–d present the real microstructure, the two phases (black: Fe, white: copper), the grains, and the finite element mesh with the refined meshing on the grain boundaries, respectively. The characters A and P in Fig. 3c present the copper and the iron grain which surround them, correspondingly. Initially, all elements in a certain grain have the same orientation. Grain orientations for arbitrary two grains are different.

Table 1 lists the information about the number of the identified iron and copper grains, the total number of elements, and the element type used in the simulation of the Fe17–Cu83 and the Fe50–Cu50 composite (Fig. 2c and d and Fig. 3c and d).\(^3\)

The volume fraction of the iron phase is 22% and 49% in the simulation for the above mentioned two composites. The element type applied in the simulation is CGAX3H which belongs to the generalized axisymmetric solid element [1]. Due to the automatic mesh refinement on grain boundaries, the meshing could not provide a corresponding node on the opposite side for each boundary node. Therefore, the application of the periodic boundary conditions has not been made. Strain-based homogeneous boundary conditions are used.

4.2. Material parameters

The velocity gradient \( L \) is assumed to be constant which means that the material structure is loaded under a constant strain rate
and spin. $F(t) = \exp(\mathbf{L}t)F_0$ is the relation between $F$ and $\mathbf{L}$. In Table 2, three independent constants in the elasticity tensor $\mathbf{C}$ are presented for both the copper and the iron phase [6].

Input parameters of composites are obtained by fitting the experimental $\sigma - \varepsilon$ curves under simple compression load (see Fig. 4) by the Taylor model. For Figs. 2 and 3, the position of the cutouts with respect to the axisymmetric axis is given in Fig. 5, where the loading direction is the $X$-direction. Table 3 exhibits the input parameters identified from Fig. 4. $\gamma_0$ is chosen as $10^4$ s$^{-1}$ [11]. The initial orientation of each grain is randomly given, since there is no preferred orientation for the grains before the tests. Schneider [15] provides more information about the identification process.

5. Results and discussion

5.1. Local deformation behaviour of grains

The overall elasto-plastic behaviour of inhomogeneous materials, like Fe–Cu polycrystals, can be strongly influenced by local incidents such as the initiation and the propagation of the shear bands, recrystallization processes, the grain geometry, and the orientation. During simulations with a simple compression load, it is
observed that the rotation and the displacement of the small harder phase particles are strongly influenced by the grain orientations. This influence is caused not only by the orientation of the particle itself but also by those of its neighbouring grains and particles. The Fe17–Cu83 composite has a large amount of the softer phase which flows around the harder phase. In the large grains, some parts which are slender or near grain boundaries are more sensitive to the change of the crystallographic orientation than other parts. Generally, the deformation behaviour of grains or particles with large sizes varies not as much as with small ones due to different initial grain orientations.

The extra marked single Cu grain “A” in Fig. 3b is a very large grain of the softer phase, the diameter of which is approximately one-half of the total length in the transverse direction and one-third in the loading direction. This special grain is supposed to undergo even larger plastic deformations. The grain boundaries of the large iron grain “P” (see Fig. 3c) coincide with boundaries of the selected structure. This may cause some unexpected effects on the deformation of grains which is not the case in the reality. Fig. 6 shows the strain rate distribution (a) and the deformed grains (b) of the Fe50–Cu50 composite at 90% plastic strain, in which the lines present four major shear bands numbered from 1 to 4. This pattern of the shear band distribution keeps its form for the different initial grain orientation. The shear bands 2 and 4 appear very early, and the shear band 1 shows up later than the band 3 which forms at about 30% plastic strain. During the loading process, some secondary short shear bands turn up at early stages and disappear at the high plastic strains. The large Cu grain A (see Fig. 3c) is surrounded by the above mentioned shear bands. The plastic deformation of A is larger near its grain boundary than the inside region. The shear band should be the major reason to result in the above mentioned phenomenon. However, based on observations of the numerical results, the opposite deformation pattern also exists. Regions inside a large grain possibly show larger plastic deformations than regions near the boundary (e.g., the large grain P in the harder phase in Fig. 3c). This large Fe phase grain locates at the corner of the cutout and has also Cu grain neighbours, which means that its deformation is influenced by the interaction between phases and grains, the grain orientation, the boundary conditions, etc. The constraints of the geometry may be also a reason. It needs further study to clearly explain this phenomenon. The histogram Fig. 7 shows the distribution of the norm of the deviator of the strain rate \( \| D \| \) for the grain A. The extremely deformed part which corresponds to the value of \( \| D \| > 1.7 \times 10^{-3} \) localizes in the black region of the shear band 2 (Fig. 6a). In the orientation space, we define the distance of the crystal orientation from its initial

<table>
<thead>
<tr>
<th>Material</th>
<th>( \tau_0^c ) (MPa)</th>
<th>( \tau_0^v ) (MPa)</th>
<th>( \epsilon_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe/Cu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fe17–Cu83</td>
<td>405/280</td>
<td>180/70</td>
<td>780/330</td>
</tr>
<tr>
<td>Fe50–Cu50</td>
<td>403/276</td>
<td>186/80</td>
<td>830/490</td>
</tr>
</tbody>
</table>

Table 3
Hardening material parameters for Fe–Cu composites.

<table>
<thead>
<tr>
<th>Material</th>
<th>( m )</th>
<th>( \gamma_0 (10^2 \text{ s}^{-1}) )</th>
<th>( n )</th>
<th>( \gamma_0 (1.0 \times 10^{-3} \text{ s}^{-1}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe/Cu</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fe17–Cu83</td>
<td>20</td>
<td>1.0</td>
<td>46.3</td>
<td>1.0</td>
</tr>
<tr>
<td>Fe50–Cu50</td>
<td>20</td>
<td>1.0</td>
<td>46.3</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Fig. 6. Strain rate (traceless part \( D \)) distribution with shear bands (a) and deformed grains (b) at \( \epsilon_p = 90\% \) for Fe50–Cu50 composite.
one as the self-misorientation. The crystal orientation $\mathbf{Q}_t$ is specially chosen such that it maps the lattice vector $\mathbf{g}_i(0)$ at time $t = 0$ onto the lattice vector $\mathbf{g}_i(t)$ at time $t > 0$. The assigned orientation on each integration point in the simulation representatively indicates the orientation of lattices, the volume of which is presented by the volume covered by this integration point. All the integration points inside a grain have the same initial orientation. The lattice rotates and the anisotropy appears, if $\alpha = \langle \mathbf{Q}_t, \mathbf{Q}_0 \rangle$ is none zero after deformation. The mean value of the self-misorientation is an indicator for the lattice rotation. Since the mean value of the self-misorientation of the grain $A$ is increasing (Fig. 8), the anisotropy of the lattice rotation within $A$ is also amplified according to the macroscopic plastic strain.

In the experiment of Tatschl and Kolednik [18], it has also been observed that strong heterogeneities in the in-plane strain and in the local lattice rotation exist within a single grain for copper polycrystals under tension.

Fig. 9 (left column) displays the distribution of self-misorientation for the iron and the copper phase of the Fe17–Cu83 composite under the simple compression load at $\varepsilon_p = 90\%$. Compared to the copper phase, the iron phase shows a lower mean value of the self-misorientation (Fe: $\sim$15°, Cu: $\sim$17°). But the oscillation of the self-misorientation distribution is much larger for the iron phase than for the copper phase. The geometry and the distribution of the harder phase particles may be one of the reasons for such an oscillation. Since the harder phase particles with quite dissimilar sizes are embedded in the softer matrix, the flow of the copper causes the large difference of the rotation of the Fe particles. The distribution of the self-misorientation of both the iron and the copper phase for the Fe50–Cu50 composite (Fig. 9, right column) are not as smooth as that of the copper phase for the Fe17–Cu83 composite. Possibly, the strong shear bands cause the high heterogeneity of the lattice rotation. The mean value for both the iron and the copper phase of Fe50–Cu50 (Fig. 9) is higher than that of the Fe17–Cu83 composite, respectively. There is, however, not a big differ-

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**Fig. 7.** Histogram of strain rate (traceless part $|\mathbf{D}'|$) distribution at $\varepsilon_p = 90\%$ for grain “A” of Fe50–Cu50 composite.

**Fig. 8.** Mean value of self-misorientation ($\alpha = \langle \mathbf{Q}_t, \mathbf{Q}_0 \rangle$) for grain “A” of Fe50–Cu50 composite until the plastic strain $\varepsilon_p = 90\%$.

**Fig. 9.** Histogram of the self-misorientation ($\alpha = \langle \mathbf{Q}_t, \mathbf{Q}_0 \rangle$) distribution of Fe and Cu phases at $\varepsilon_p = 90\%$ for Fe17–Cu83 (left column) and Fe50–Cu50 composites (right column).
ence for the mean value of the self-misorientation between the iron and the copper phase for the Fe50–Cu50 composite.

5.2. Stress–strain flow behaviour

Since the microscopic stress–strain behaviour can be modified by the anisotropy of the grain orientation distribution, the number of grain orientations should be representatively enough to predict the stress–strain curves which are comparable with the experimental ones. In Fig. 10, the stress–strain curve is averaged from 18 calculations with different initial grain orientations for the Fe17–Cu83 composite. Since, as already mentioned in Section 4.1, the volume fraction of Fe phase is about 22% in the axisymmetric simulation, it is reasonable that the simulated stress–strain curve is located between the experimental ones of the Fe33–Cu67 and the Fe17–Cu83 composite.

Fig. 11 compares the stress–strain curves of the experiment and the FE prediction which is an average of 22 simulations with different initial grain orientations. In the Fe50–Cu50 case, the simulated curve matches also well the experimental one.

In order to show the influence of the initial grain orientation on the local flow behaviour, Figs. 12 and 13 exhibit the normalized stress–strain curves which are obtained by

\[ \sigma_N = \frac{\sigma_{\text{max/min}}(t)}{\sigma_{\text{aver}}(t)} \]

\[ \sigma_{\text{aver}} = \frac{\sum_{i=1}^{n} \sigma_i}{n} \]  

with \( n = 18 \) for the Fe17–Cu83 and \( n = 22 \) for the Fe50–Cu50 composite. \( \sigma_N \) presents the normalized stress. The maximum stress and the minimum stress are given by the simulated stress–strain curves which are located at the highest and the lowest position among all the simulations, correspondingly. The deviation from the averaged stress–strain curve is about 1–2% for the minimum stress–strain curve (dashed line in Fig. 12) of the Fe17–Cu83 composite while it is about 5% for the maximum stress–strain one. This 5% deviation remains true for the maximum and minimum stress–strain curves for the Fe50–Cu50 composite (Fig. 13). Different orientation distributions of grains may cause 5% fluctuation for the local stress–strain curves, if a relatively small number of grains\(^3\) is considered in the microstructure in the axisymmetric simulation.

Fe–Cu composites exhibit an increased stiffness (compared to the pure copper) and ductility (compared to the pure iron). The phase stress partition, i.e., the softer phase transfers the load to the harder phase, is the reason for the former property. Figs. 14 and 15 show the normalized stress flow in each phase for the Fe17–Cu83 and the Fe50–Cu50 composite, respectively. \( \sigma_{\text{phase}} \) and \( \sigma \) present the stress for the Fe or the Cu phase and the total stress, whereas both stresses are the averaged values from three simulations. These three simulations are chosen from the 18 (Fe17–Cu83) and the 22 (Fe50–Cu50) calculations. For a given strain, the stresses predicted by two of these three simulations give the largest and

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\(^{3}\) According to Cheong and Busso [4], such number of grains is between 10 and 100.
the smallest stress, respectively. The location of the third stress–strain curve is nearest to the averaged (stress–strain) curve among the 18 (Fe17–Cu83) and the 22 (Fe50–Cu50) calculations. We define $r_{\text{phase}}$ as the normalized phase stress. At the beginning of the yielding, the normalized strength of the iron phase decreases fast, and that of the copper phase exhibits the reverse effect for both composites (Figs. 14 and 15), whereas the rate of this decrease or increase is higher for the Fe17–Cu83 composite than for the Fe50–Cu50 composite. This trend diminishes with the increase of the plastic strain. At last, the normalized phase stress converges to a certain value which varies according to the ratio of (Fe:Cu) phase volume fractions. At the beginning of the yielding of the composite, it is observed that the iron phase starts to yield partly in experiments [5]. On the other hand, some iron phase is still in the elastic–plastic transition up to higher macroscopic strains [6]. This means that the plastic deformation of the iron phase takes place step by step. If the harder phase yields, the load will be transferred back to the softer phase [7]. As a result, the normalized stress of the iron phase decreases, while the normalized stress of the copper phase shows the opposite effect with an increase of the plastic strain. The observations in the experiment prove that the numerical results in Figs. 14 and 15 are reasonable for the phase stress flow behaviour.

5.3. Crystallographic texture

The crystallographic textures are presented as inverse pole figures, which are obtained from 18 and 22 calculations for Fe17–Cu83 and Fe50–Cu50 composites, respectively. The iron phase texture presented as the standard inverse pole figure is indicated in Fig. 16 for both the simulation and the experiment at 90% plastic strain under compression load. Two fiber components, (100)–fiber and (111)–fiber are observed, which are typical for compressively deformed $\alpha$-Fe [12]. Such a fiber texture is well captured by the simulations for both the Fe17–Cu83 and the Fe50–Cu50 composite. The prediction also demonstrates the difference of the fiber intensity due to the phase volume variation, even though the maximum value of the fiber intensity is slightly higher in the Fe50–Cu50 than in the Fe17–Cu83 composite. While the experiment shows approximately the same fiber intensity. Since each inverse pole figure includes more than 600 orientations which are initially assigned randomly to the grains, the effect of the local grain orientations on the texture can be neglected. In this case, the local interaction and the phase arrangement are two major factors influencing the texture evolution in the simulation. Due to the limited number of grains in both real microstructures considered, the amount of the local interaction should be also approximately the same. In this case, the influence of the local interaction on the texture shown here is a minor factor, which causes the higher fiber intensity in the Fe50–Cu50 composite. The particle distribution of the Fe50–Cu50 composite may result in a higher fiber intensity than that of the Fe17–Cu83 one, since such distributions lead to
an even stiffer material structure in which four large iron particles are located on the structure boundaries.

The simulated and the experimental texture of the copper phase is given in Fig. 17 for the Fe17–Cu83 and the Fe50–Cu50 composites. In the simulated textures, the pronounced $h_{110}$-fiber develops to the $h_{411}$ direction. A rather soft texture of the Cu phase is presented by the measurement for the Fe50–Cu50 composite, which is not well simulated by the FE model. Besides the above mentioned reasons, i.e., the local interaction, the limited material structure, and the boundary conditions, the present model may not be able to catch the local change of the activation of the slip systems rapidly enough due to the isotropic hardening assumption.

5.4. Local strain distribution

The anisotropy of the constituent grains causes high heterogeneities in the local strain field when the polycrystalline structure is under load. We analyzed the local strain for both the iron and the copper phase at a 19.8% tensile plastic strain. Fig. 18 presents the histogram of the local plastic strain for the Fe50–Cu50 composite, which is not well simulated by the FE model. Besides the above mentioned reasons, i.e., the local interaction, the limited material structure, and the boundary conditions, the present model may not be able to catch the local change of the activation of the slip systems rapidly enough due to the isotropic hardening assumption.

Both the distribution and the mean value of the plastic strain match the reality well for the iron phase in all the mentioned directions. The strain of the iron phase behaves more heterogeneously in the loading direction (LD) than in the shear direction (LD/TD) due to the wider range and the larger oscillation of the distribution curve in the LD direction, while this nonhomogeneity lies in the middle for the transverse direction (TD). Since there is neither a residual stress nor a residual strain before loading, a wider range of the strain distribution in a given direction means a stronger dispersion of the local strain, i.e., the material deforms more heterogeneously in this direction. The mean value of the plastic strain is 16.99% in the loading direction for the simulation and 15.3% for the experiment. Both values are much smaller than the mean value of the composite (19.80%). These mean values are −7.1% and −7.0% for the transverse direction in the numerical and the experimental predictions, correspondingly. There is no obvious deviation of the mean value from the total one for the shear direction. Generally, the absolute mean value of the plastic strain for the harder iron phase is less than that of the composite.

For the copper phase, the experiment (in Fig. 18) clearly presents a wider range of the strain distribution in the loading direction than in the other two directions, i.e., there is more inhomogeneity in the LD direction. This property is well predicted by the numerical simulation. In the loading direction, the numerical curve even captures the second peak shown at approximately 27% plastic strain in the experiment. The mean value of the copper phase plastic strain is 20.8% in the simulation and 20.9% in the experiment. The corresponding results for the TD directions are 10.6% for the FE prediction and 9.1% in the experiment, respectively. Like in the iron phase, this value is still approximately zero for the shear direction (LT/TD). Contrary to the harder phase, the mean value of the plastic strain for the Cu phase is higher than that of the total composite. This corresponds to the general conclusion for the two-phase polycrystal mechanical behaviour, i.e., the softer phase burdens more deformation than the harder one.

6. Summary

In order to understand the mechanical behaviour of the Fe–Cu composites and, particularly, the coupling of the microscopic and the macroscopic deformation behaviour under large plastic deformations, axisymmetric simulations have been performed by the finite element software ABAQUS. The elasto-viscoplastic material model has been applied. Material structures are modelled based on real microscopic cutouts, in which regions near grain bound-
aries are finer meshed than other parts. Two composites, Fe17–Cu83 and Fe50–Cu50, are taken as representative microstructures which are investigated in detail. From the investigations of the local deformation, the flow behaviour, the texture, and the distribution of the strain, we draw the following conclusions:

- The self-misorientation of the large grain in the copper phase is amplified according to the increase of the macroscopic plastic strain, whereas self-misorientation is defined as the deviation of the crystal orientation from its initial one. There is only a slight difference between the mean value of self-misorientation in the iron phase and that in the copper phase.
- In case the local stress is influenced only by the initial grain orientations in a given microstructure, i.e., all other conditions are kept identical in the simulations, a deviation of 5–10% can be observed for the local stress normalized by the macroscopic stress.
- The stress–strain behaviour is well captured for both Fe–Cu composites mentioned. The stress of each phase is sensitive to the amount of the plastic deformation at the early stage of the yielding. The normalized stress in the iron phase decreases fastly, and that in the copper phase shows the reverse effect.
- The simulated texture of the iron phase describes well the fiber type texture and the (maximum) fiber intensity variation according to the volume change of phases. The predicted texture of the Cu phase also captures the experimental fiber texture in the microstructure for the simulation, the Fe50–Cu50 composite, while no obvious difference is shown in reality.
- Concerning the distribution of the plastic strain (Fe17–Cu83 composite), the mean value of the strain in both the harder phase and the softer phase presents a deviation from the total mean value in the normal and the transverse direction. The copper phase undergoes larger deformations than the iron phase in the composite. These properties are well predicted by the axisymmetric simulation.
- The mean value of the strain is quantitatively well predicted for both the iron and the copper phase.

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References