3D Analysis of MMC microstructure and deformation by $\mu$CT and FE simulations

Horst-Artur Crostack$^a$, Jens Nellesen$^b$, Gottfried Fischer$^b$
Siegfried Schmauder$^c$, Ulrich Weber$^c$, Felix Beckmann$^d$

$^a$TU Dortmund, Department of Mechanical Engineering,
Chair of Quality Management, D-44221 Dortmund, Germany;
$^b$RIF e.V., Joseph-von-Fraunhofer-Str. 20, D-44227 Dortmund, Germany;
$^c$Institute for Materials Testing, Materials Science and Strength of Materials,
University of Stuttgart, Pfaffenwaldring 32, D-70569 Stuttgart, Germany;
$^d$GKSS-Research Lab., Max-Planck-Str. 1, D-21502 Geesthacht, Germany

ABSTRACT

A better understanding of micro deformation and damage processes that the microstructure of particle reinforced metal matrix composites (MMC$_p$) undergo at microscale before macroscopical failure gives the right direction for the microstructural design of these materials. To this end, a $\mu$CT-based analysis was performed that combines $\mu$CT-experiments and FE simulations:

The gauge length of tiny tensile specimens (cross-section $A = 2 \times 1 \text{ mm}^2$) consisting of the MMC$_p$ systems Cobalt/Diamond and Al/B$_4$C was imaged by tomography at different stage of deformation. 3D strain tensor fields and displacement vector fields were determined by digital image correlation of the reconstructed tomograms. Based on tomograms of the analysed volume at the undeformed state, FE meshes were generated that model the microstructure close to reality. Using these meshes and the displacement vector fields measured at the volume boundaries, FE simulations of the deformation and damage behaviour were carried out. In both composites volume strains below 1% have been found experimentally. The spatial resolution of deformation fields is limited by the characteristic microstructural length which depends on the particle diameter and the particle spacing. The results of the experiments and the simulations are compared on the basis of 3D-strain fields sampled within the analysed microstructural region. Additionally, the impact of microstructural features on the localisation of strain, the initiation of localised damage and the successive failure of the composite materials is discussed.

Keywords: X-ray microtomography, FEM, MMC$_p$, Micromechanics, Damage

1. INTRODUCTION

The localisation of strain in metallic materials is of great practical interest, since this process plays an important role for the locus and the type of the successive failure of a component. Moreover, the behaviour during machining is influenced by this process. In addition, strain localisation can lead to undesired roughness of the surface of sheets and diminishes fracture strain. In order to affect this strain localisation in the framework of material optimisation knowledge about the effects of alloy composition, precipitation state, microstructure and loading conditions (strain rate, temperature, multiaxiality, ...) is needed. In case of reinforcement of a metallic material by dispersion of brittle particles the impact of volume (fraction), shape, orientation and arrangement of the particles on the localisation has to be considered accessorially. In the case of composites the different mechanical behaviour of the phases and the actual condition of the phase interfaces has to be taken into account.

With non-destructive testing methods microstructure can be mapped in different load stages to uncover strain localisation which does modify microstructure.

Further author information: (Send correspondence to J.N.)
J.N.: E-mail: Jens.Nellesen@rif-ev.de, Telephone: +49 (0)231 755 5473
U.W.: E-mail: Ulrich.Weber@mpa.uni-stuttgart.de, Telephone: +49 (0)711 685 63055
In the past most investigations concerning the deformation and damaging behaviour of multi-phased materials were confined to the accessible specimen’s surface. With incoherent and coherent optical methods or scanning electron microscopy in-situ measurements of deformation and damaging were carried out with high magnification.\textsuperscript{1,2}

An improvement of this methodology was achieved by measuring the deformation field: For this purpose the microstructure (which was artificially textured by lithographic methods additionally) was imaged in different load states and afterwards these images were analysed by digital grey value correlation. Moreover, these experimentally obtained images of microstructural areas and the displacement vector fields at their boundaries were used to set up FE models with phase structures and boundary conditions close to reality.\textsuperscript{3}

In order to study the processes with high time resolution high-speed CMOS cameras were applied.\textsuperscript{4,5} The authors of this work also developed a technique which relies on the computation of temperature images acquired with a high speed infrared camera.\textsuperscript{6,7} However, the differences in the results of 2D FE simulations and 2D experiments reveal the limitations of these 2D approaches: Microstructural objects underneath the specimen’s surface which do influence the deformation process cannot be taken into consideration. Furthermore, phase regions which appear to be disjoined at the surface can be connected in the subsurface region.

Due to the described restrictions of the 2D analysis the authors favour the deformation and damaging analysis in the bulk of the specimen by means of non-destructive micro computer tomography: In different load or deformation stages 3D-images of the microstructure are created. Utilising the attenuation contrast between the phases, these images are evaluated with the above mentioned correlation algorithm, which was extended to the third dimension to compute 3-dimensional strain and displacement fields in the bulk of specimens.

3D FE models generated on the basis of the tomograms are used to simulate the material behaviour by FE calculation. From the comparison between the experimentally observed and the simulated behaviour and results of parameter studies better understanding of the localisation process can be deduced.\textsuperscript{8}

In contrast to the correlation algorithm developed by the authors which exploits grey level gradients, HALDRUP ET AL.\textsuperscript{9} determine the grey value weighted centers of gravity of individual particles which were used to calculate the displacement gradient tensor of each particle by a least squares fit of the relative displacement of the eight nearest neighbour particles.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Comparison of microstructure of different particle-reinforced metal matrix composites, composite with 300 $\mu$m (left column) and $\approx 90$ $\mu$m diamond particle size (right column).}
\end{figure}
In the work of VERHULP ET AL.\textsuperscript{10} tomographically obtained microstructure (of bone tissue) is transferred to a tetrahedra mesh. The displacements at the tetrahedra nodes and from this the deformation tensor of each tetrahedron are computed on the basis of the tomograms. Comparisons with FE simulations are not conducted.

2. MATERIALS AND METHODS

2.1 Materials and experimental procedure

In the scope of the studies particle-reinforced metal matrix composites have been investigated which are used for cutting segments of rotating tools for stone machining. Two different commercially available segments consisting of a cobalt matrix with dispersed diamonds and WC-particles have been studied. Tiny dog-bone shaped tensile specimens with a cross-sectional area $A = 2 \text{ mm}^2$ were manufactured by water jet cutting. Experiments were performed at beamline HARWI-II in HASYLAB at DESY, Hamburg, Germany with monochromatic photons (energy $E = 82$ keV and $E = 100$ keV, respectively). At a glance, the differences in microstructure between both materials can be spotted in fig. 1. In the two-dimensional tomogram region on the left only two large diamonds are visible. The diameter of the diamonds averages about 300 $\mu$m. The composite on the right contains quite a lot diamonds (dark) with a mean diameter of approximately 90 $\mu$m.

Moreover, the particle-reinforced metal matrix composite Al/B$_4$C was investigated which was manufactured by plasma spark sintering. The composite mainly consists of high-purity (99.99\% Al) aluminium which shows a ductile behaviour. In this matrix brittle B$_4$C-particles are dispersed whose mean particle diameter amounts to...
Figure 3: Displacement vector field acting upon the model boundaries; before (left hand side) and after (right hand side) splitting off the rigid body rotation.
Figure 4: Comparison of microstructure of different particle-reinforced metal matrix composites and colour-coded overlaid distribution of equivalent strain $\varepsilon_{\text{equ}}$, composite with 300 $\mu$m (left column) and $\approx$ 90 $\mu$m diamonds (right column)

this means a rough mapping between both tomograms is given. On the basis of this a-priori information a radiometric transform

$$g_t(x, y, z) = r_0 + r_1 \cdot g_v(x_t, y_t, z_t)$$

and an affine transform

$$x_t = a_0 + a_1 x + a_2 y + a_3 z$$
$$y_t = b_0 + b_1 x + b_2 y + b_3 z$$
$$z_t = c_0 + c_1 x + c_2 y + c_3 z$$

are iteratively optimised to map the start cuboid best possible onto its corresponding more or less deformed microstructural hexahedral region. The residual cuboids are evaluated automatically having initialized their transform parameters by parameters interpolated from vicinal, already analysed cuboid regions.

From the affine transform the mean deformation gradient $\mathbf{F}$

$$\mathbf{F} = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}$$

and subsequently the Lagrangian strain tensor $\gamma$

$$\gamma_{ij} = \frac{1}{2}(F_{ki}F_{kj} - \delta_{ij}) \quad (1)$$

are computed. Computing this transformation for all regularly distributed cuboid regions in the tomogram yields the Lagrangian strain tensor field sampled on a discrete grid. Moreover, the strain tensor and the displacement vectors can be calculated at arbitrary positions in space. From the displacement vectors the rigid body
translation and rotation can be split off. This is important if the orientations and positions of a specimen in the tomograms differ due to experimental shortcomings during fixing the specimen to and removing it from the rotational stage of the CT scanner. Different magnifications of the specimen can also be taken into account, thereby. In fig. 3 the result of this decomposition is visualised drawing on the example of a sub-tomogram (ROI = region-of-interest) of the Co/WC/diamond composite with the larger diamonds shown in fig. 1. This ROI contains only one large diamond (cf. fig. 3). The interface between the matrix and this diamond is approximated by a surface net consisting of triangles. The diamond faces can clearly be recognised. On the left hand side of this figure the displacement vectors acting upon the boundaries of this sub-tomogram are drawn in without splitting-off the rigid body rotation. The superimposed rotation can clearly be seen. After splitting-off this rotation the vectors at top and bottom face of sub-tomogram are aligned with the direction of global load, preferentially, indicating an elongation. The vectors in the middle of the front, back, left and right faces of the ROI point to the center of the sub-tomogram indicating a contraction perpendicular to the direction of global loading.

From the Lagrangian strain tensor \( \gamma \) (equation (1)) the equivalent strain \( \varepsilon_{equ} \), a scalar quantity, can be derived after the principal axis transformation, where the trace entries \( \gamma_i \) of the diagonalised matrix are related to each other.

\[
\varepsilon_{equ} = \frac{1}{3} \sqrt{(\gamma_1 - \gamma_2)^2 + (\gamma_1 - \gamma_3)^2 + (\gamma_2 - \gamma_3)^2}
\]

The spatial distribution of the composite phases in the sub-tomogram and the displacement vector at its surface constitute the input for 3D FE model used to simulate the material behaviour. A detailed discription how to convert a 3D tomogram to a geometric FE mesh can be found in [8].

### 3. RESULTS AND DISCUSSION

The experimental studies of the authors aim at sampling strain with the highest possible spatial resolution, i.e. minimum cuboid dimensions and spacing that are influenced by the characteristic microstructural length of material. In order to investigate this effect, two commercially available composites with the same chemical composition (Co, WC and diamond) but with different particle sizes and spacings were chosen. The differences in microstructure can be seen clearly in fig. 1 and have already been discussed in subsection 2.1.

Since the strain analysis algorithm makes use of markers the lower limit of the cuboid dimensions corresponds to the mean distance between the dispersed particles. For both composites the mean distance between the WC-particles (bright, diameter \( \approx \) few microns) is smaller than the one between the diamonds (cf. fig. 1). For the composite with the smaller diamonds (right-hand side of fig. 1) the cuboid dimensions can be chosen approximately four times less than for composite with the few diamonds (left part of fig. 1).

In the first case (left column) the cuboid dimension is 42\(^3\) voxels and the spacing between the cuboid centers is 8 voxels. The voxel edge length amounts to roughly 10 \( \mu \)m. For the second composite (right column) the cuboid (also formed like a cube) has an edge length of 32 voxels. The spacing is 12 voxels. The effective voxel edge length amounts to 3.3 \( \mu \)m. The size of the images in the left column is 121 * 241 voxels whereas the width and height of pictures in the right column amounts to 585 and 511 voxels, respectively.

The comparison of the colour-coded maps of equivalent strain \( \varepsilon_{equ} \) which are overlaid over the images of microstructure reveal that regions of elevated strain can be found mostly in the neighbourhood of the diamonds. Due to the relative large dimensions of the cuboids the strain field is smoothed and therefore, high strain values can also be seen inside the diamonds in some places, which is not expected in view of the brittleness and high Young’s modulus \( E \) of diamond.

The specimen made of the cobalt/WC/diamond composite with the smaller diamonds was subjected to tensile deformation for four times. In fig. 5 the spatial distributions of equivalent strain calculated from tomograms of the second, third and fourth deformation step are visualised. Already in the second deformation step zones of elevated equivalent strain can be discovered in the top \( xz \)-plane, which retain their position but increase their value in the third and fourth deformation step.
The cuboid dimensions and spacings were varied for the second composite (right column in fig. 1) in order to study their influence. In fig. 6 the colour-coded distributions of equivalent strain $\varepsilon_{equ}$ sampled with different cuboid dimensions and spacing are displayed. The upper left picture was calculated with a cuboid size of $32^3$ voxels and cuboid grid spacing of 12 voxes whereas the corresponding values in the lower right image amount to $42^3$ voxels (size) and 16 voxels (spacing). Both distributions agree very well: Regions of elevated strain occur at nearly the same positions bearing in the mind the spatial resolution given by the cuboid spacing. Also the magnitudes of equivalent strain in both distributions resemble each other, too.

The FE software ABAQUS$^{13}$ was used to simulate the material behaviour in a ROI of the composite with the coarse diamonds utilising the experimentally obtained phase distribution and the displacement field at ROI boundary. Since standard tetrahedral elements with 10 nodes are prone to shear locking and volumetric locking the modified tetrahedral element C3D10M was selected which features a robust deformation behaviour.

The 3D distribution of equivalent strain $\varepsilon_{equ}$ was selected to compare the experimental results and the findings of the 3D FE simulation (cf. fig. 7). For different planes given by their voxel index a colour-coded representation of equivalent strain is depicted in this figure. Diamonds in the bulk which are intersected by these planes are indicated by their perimeters.

The results agree fairly well: Since diamond deforms purely elastic no plastic strain can be found in diamond in the FE simulation. This is indicated by blue colour of the diamonds in the simulation results (right column of figure 7). By contrast, diamonds cannot be localised precisely on the basis of differences in strain due to the relative large dimensions of the cuboids in comparison with diamond size. During tesselation of the equivalent strain phase interfaces are disregarded.

Figure 5: Localisation of strain in the course of 3 deformation step; zones of elevated equivalent strain can already be discovered in the second deformation step; these zones retain position but the strain increases with incremented deformation.
The magnitudes of equivalent strain are quite similar. Even equivalent strain $\varepsilon_{equ}$ below 1% can be quantified experimentally. However, in the simulations larger regions of high equivalent strain (red areas) are visible. This discrepancy can be caused by the fact that the three-phased composite was restricted to the two components cobalt and diamond in order to simplify the simulations. In future work, the complete three phase system including the WC particles will be simulated on the one hand. On the other hand the two phase system cobalt/WC will be considered as a homogeneous matrix simulated with effective material parameters.

The second selected MMC-system (Al / B$_4$C (cf. subsection 2.1)) is better qualified for deformation analysis due to the high ductility of the Al matrix and the dense distribution of the dispersed B$_4$C particles. In order to provoke damaging in the gauge length the tensile specimen was notched on two sides.

From the right 2D-image ($xz$-slice) in fig. 8 extracted from the 3D-tomogram it is obvious that a crack which was initiated at the right notch propagates through the specimen. A visual inspection of the vicinal $xz$-layers revealed that the crack might be caused by an agglomeration of particles in the neighbourhood of the right notch. Although the left notch is a little bit deeper the crack originates from the base of the right notch. Accordingly, the colour-coded 3D distribution of equivalent strain $\varepsilon_{equ}$ (cf. fig. 9) shows a strain concentration in the neighbourhood of the right notch already in the third stage of deformation.

Up to now deformation was represented by the scalar equivalent strain $\varepsilon_{equ}$ (equation (2)). This scalar is derived from the Lagrangian strain tensor $\gamma$ which can be depicted by an ellipsoid oriented in space and scaled according to its eigenvalues and eigenvectors. The representation of the Lagrangian tensor field with ellipsoids gives an improved insight in localisation of strain. In fig. 10 this tensor field in the notched tensile specimen made of the Al/B$_4$C composite is rendered in this manner utilising the VTK-library. At a glance, the plastic flow around the notches can be recognised. Especially, at the base of right notch where the crack is initiated very large ellipsoids are found corresponding to the elevated value of equivalent strain $\varepsilon_{equ}$ (cf. the strain distribution for the fourth deformation step in fig. 9). Also the pattern of bigger ellipsoids coincides with greenish bands indicating moderate strain in this subfigure.
Figure 7: Comparison of the distribution of equivalent strain $\varepsilon_{equ}$ in the cobalt/WC/diamond composite after maximum deformation in different cross sections: experiment (left column), FE simulation (right column), (cross sections are given by the constant tomogram coordinate (voxel index))
Figure 8: 2D-images of microstructure from the bulk of a notched tensile specimen consisting of the Al/B₄C-composite in different stages of deformation representing nearly the same microstructural region; no deformation (left); advanced deformation and damage initiation (right)

Figure 9: Colour-coded 3D-distribution of equivalent strain $\varepsilon_{equ}$ in the gauge length of the notched tensile specimen at the third deformation step; elevated strain can be found in the vicinity of the notch bases, especially in the region of the right notch where a crack is initiated.
Figure 10: 3D representation of the field of Lagrangian strain tensors $\gamma$ with ellipsoids; the middle plane in the gauge length of the notched tensile specimen consisting of Al/B$_4$C at the fourth deformation step is shown.

In this case the strain concentration can be related to the notch effect and the crack initiated at the notch base. However, strain concentrations were also found in unnotched and uncracked specimens made of the same MMC. The microstructural causes (agglomeration of particles, particle-free zones, ...) of these localisations processes will be subject of future studies.

ACKNOWLEDGMENTS

For assistance during measurements at beamline HARWI-II of HASYLAB at DESY, Hamburg, Germany we would like to thank J. Herzen.

Part of this work was financially supported by the German Research Foundation (DFG) in the scope of projects no. CR 4/111-2 and SCHM 746/54-2 which is gratefully acknowledged.

REFERENCES


