Tomographic Analysis and FE-Simulations of MMC-Microstructures under Load

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ABSTRACT

Microstructural changes like micro deformation and damaging due to tensile load precede the macroscopical failure of a component. In order to contribute to the understanding of such processes, the microstructure of tensile test specimens was imaged by microtomography in the course of deformation.

The specimens consist of particle reinforced metal matrix composites (the MMCs Cobalt/Diamond and Al/TiN) manufactured on a powder metallurgical route. Tomograms of a volume in the gauge length of the specimens were reconstructed from the projection data acquired at different deformation stages. Both polychromatic radiation of a microfocus X-ray tube and monochromatic synchrotron radiation were used for projection data acquisition.

With the help of 3D data processing 3D surface nets were extracted from the tomograms which indicate the particle/matrix interface. These nets which are composed of triangles were afterwards optimized with respect to the shape of the triangles. Using the triangles as seeds a 3D FE-mesh without gaps consisting of tetrahedra was generated. 3D FE-simulations were carried out utilizing both arbitrary and realistic boundary constraints. Realistic conditions were derived from an iterative matching procedure of tomograms. The effect of finite element type (tetrahedron or hexahedron) on the simulated distribution of stresses was analyzed. The appearance and development of plastic zones in the metal matrix depending on externally applied displacements were studied in the simulations. The calculated peak stresses are compared with the loci of cracks found in the tomograms.

Keywords: X-ray microtomography, FEM, MMC, Micromechanics

1. INTRODUCTION

During plastic deformation of metallic materials strain concentrations (e.g. plastic zones, shear bands, PLC bands) and micro damages occur. Understanding of such micro processes which run before the specimen fractures can be deduced by an approach which combines experimental analysis and FE-simulation. In the framework of experimental analysis the microstructure is sampled at different stages of the loading course with imaging techniques. Based on the results of the imaging techniques a model of the microstructure can be set up. Utilizing this model the material behavior is simulated then. In this manner, FE-simulations can be performed which are close to reality. In a different approach the microstructure is simplified by a unit-cell model\textsuperscript{1,2}

Chawla et al.\textsuperscript{3} derived FE-models from serial sectioning of a specimen. With this technique microstructures can be imaged only at one deformation stage. For this reason, non-destructive techniques should be used for rendering the microstructure of a specimen in several stages of deformation or load.

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In 2D a couple of non-destructive experimental techniques were deployed to study deformation fields and strain localization processes using incoherent and coherent optical methods, scanning electron microscopy and thermography. The variation of microstructural features and their arrangements and the changing of superficially applied grids or patterns were utilized for the observation of plastic deformations. However, the necessary sample preparation can spoil the strain fields. Furthermore, microstructural objects and deformation processes beneath the specimen’s surface can not be imaged by these ‘surface’ techniques and, therefore, can not be taken into account in comparing 2D FE-simulations.

For this reason, X-ray tomography also known as computed tomography (CT) is increasingly applied to characterize microstructural features and processes in the bulk of materials. In order to achieve the necessary high spatial resolution in the micrometer range, two techniques are qualified which differ in the radiation source. Firstly, absorption tomography with X-rays emitted by a micro-focus tube can be performed. Secondly, with X-ray tomography microscopy (XTM), in which synchrotron light is used to penetrate the specimen, a high contrast resolution in the tomograms can be accomplished due to the monochromaticity of the radiation.

Besides absorption tomography also phase-contrast tomography was used to image microstructures with low attenuation contrast.

In the last years, different techniques have been implemented to study displacement and strain fields in the bulk of materials starting from tomograms. Nielsen et al. identified several particles in the tomograms at different load stages. In the gray scaled tomograms the gray-value-weighted centers of gravity of each particle were determined, 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 neighbor particles.

The authors of this work developed a matching algorithm which maps corresponding tomogram sub-volumes of different deformation stages onto each other by a combined radiometric and geometric (affine) transformation. After an iterative optimization of these transforms the Langrangian strain tensor and the displacement are computed from the affine transform.

This experimental technique was used to deliver input data for 3D FE-simulations. From the information about the microstructure realistic two-phase FE-models were generated, which include the spatial distribution of the material phases, the material properties and the displacement vectors at the model surface serving as boundary conditions. The behavior of microstructure was simulated on the basis of this model then.

In a previous report the microstructure of the system Al/TiN was modelled using brick elements. Meanwhile, the FE-meshes are generated on the basis of three-dimensional triangle nets, which mark the phase boundary. These nets are derived from the tomograms and optimized with respect to the shape of triangles. The method was tested on the systems Al/TiN and Co/Diamond.

2. MATERIALS AND METHODS

2.1. Materials and specimens

Two particle-reinforced metal matrix composites (MMCs) were studied. The commercially available system Co/WC/Diamond consists of Diamond and WC particles which are dispersed in a Cobalt matrix. This material is widely used for rotating tools cutting stone. The self-made metal matrix composite Al/TiN was produced on a powder metallurgical route. Tiny plain dog bone shaped tensile specimens were prepared from these materials by water jet cutting and spark cutting, respectively (cf. Fig. 1).

2.2. CT-Data Acquisition

Part of the experiments with the MMC Cobalt/Diamond were performed at beamline HARWI-II in the HASY-LAB at DESY, Hamburg, Germany using monochromatic photons of 82 keV which were selected by a double-crystal monochromator in Laue-arrangement from the white beam. Due to the well fulfilled approximation of parallel beam geometry projection data were acquired at 720 rotation angles which were uniformly distributed in the semi circle. The other radioscopic images were taken with a CT-scanner, which is composed of a Scannray micro-focus tube MFT150, a four-axes specimen holder (to move the specimen along the axes of a Cartesian coordinate system and to rotate the sample) and a flat-panel detector (RID 512-400, EG&G Heimann). During
Figure 1. Stress-elongation curve and distribution of equivalent strain $\varepsilon_{\text{equ}}$ at the specimen’s surface after fracture (b) obtained by matching the SEM-images (a) and c)); relationship between high strain and cracking, see macro crack (c) and micro cracks in d) and e).

the discontinuous scanning the specimen was rotated 360 times inside the cone-beam with an increment of 1°. The maximum accelerating voltage of 150 kV was chosen.

2.3. Reconstruction
A modified version of the DONNER-library was used to reconstruct the tomograms from the parallel beam projection acquired with synchrotron radiation. This version allows to take into account an offset angle during reconstruction. The BKFIL-routine (backprojection of the filtered projection) was applied to perform a 2,5D reconstruction i.e. a slice-by-slice reconstruction which yields a stack of 2D-slices.
A cross-platform reconstruction algorithm was developed in order to reconstruct cone-beam data which is based on the so-called FELDKAMP reconstruction formula. Overall reconstruction times of about half an hour for a reconstruction of $512^3$ voxels from 360 projections were achieved on a Quad-Pentium III 700 MHz by data partition and parallelizing the code utilizing the POSIX thread library. Only the voxels inside the cylinder inscribed in the reconstruction cube were taken into account.

3. EXPERIMENTAL PROCEDURE AND RESULTS

With SEM the specimen’s surface was recorded in the undeformed stage and after fracture (cf. the stress-elongation curve in Fig. 1). The surface reveals both diamonds and holes where diamonds were located formerly (cf. Fig. 1a), d), e)). After fracture, micro cracks originating from diamonds resp. holes could be found (cf. Fig. 1d), e)). Before the tensile test the surface was artificially structured by an applied gold dot grid (see Fig. 1a) and e)) to get additional gray level gradients in SEM-images. On the basis of the gray level gradients an iterative matching of sub-images of different stages of deformation was carried out (image correlation). From the local transformation matrices describing this local mapping the field of equivalent strain was calculated. The field was overlaid semi-transparently on the SEM-image in Fig. 1b)). Strain concentrations emerge in areas of microcracks which are initiated in the neighborhood of diamonds and holes.

By SR-based tomography the microstructure of a Co/Diamond composite was uncovered as depicted in Fig. 2. The shape of diamonds in the bulk of the specimen can easily be recognized (cf. Fig. 2b)). The distribution of the smaller WC inclusions can be visualized by making the matrix completely transparent (cf. Fig. 2c)).

4. DATA ANALYSIS

4.1. Change of particle distances

In principle, distance variations between diamonds and WC particles can be evaluated to get quantities characterizing local deformation. Both brittle phases show good contrast to the Co matrix in the tomograms.
comparison to the specimen’s cross-section the diamond particles have, however, a quite huge diameter (300 µm on the average) and only a few diamonds can be found in the gauge length of the specimen. Since it is hardly possible to determine a variation of distances between diamonds, the changes of distances between WC particles were evaluated instead. To segment the WC phase the tomogram was firstly binarized into the matrix including the WC particles and diamonds with surrounding air by applying a global threshold. Afterwards the regions in the original tomogram revealing the diamonds and the air were filled with the mean gray value of the matrix. By an adaptive threshold technique the WC-particles were segmented then. The found particle phase was labelled by 3D-region growing. Particles which are intersected by sub-volume surfaces were rejected during region growing. The center of gravity, the volume and the perimeter of the labelled particles were also calculated. If the voxel which includes the center of mass of a particle belongs to this particle, this particle is also declined. By this criterion ring artifacts can be removed which were otherwise marked as particles.

To identify a particle in tomograms revealing the microstructure in different deformation stages, the following procedure was implemented: At first, a couple of particles were identified visually. Afterwards, a mean affine 3D transform for the centers of mass was computed by means of least-squares-fitting. On the basis of this transform the remaining particles were found by mapping their centers of gravity from the undeformed state to the deformed one and searching for a center of mass in a spherical region around this transformed point. In doing so, a mapping function could be established, which naturally is not bijective or undefined in several cases.

4.2. Displacement and strain field

To compute the strain field in a microstructural region-of-interest (ROI) cubic sub-volumes (so-called cubes) of the tomogram of the undeformed state were mapped onto a hexahedral microstructural region of the tomogram of the deformed state.

For this mapping procedure an affine (equation (1)) and a gray value transformation (equation (2)) were applied utilizing three-dimensional gray value gradients within the cubes of the region. The transforms were iteratively optimized by least-squares-fitting. The Langrangian strain tensor \( \gamma \) is given by the deformation gradient \( F \) (equation (3)) which can be computed from the affine transform matrix.

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

\[
g_v(x, y, z) = r_0 + r_1 \cdot g_v(x_t, y_t, z_t) \tag{2}
\]

\[
\gamma_{ij} = \frac{1}{2}(F_{ki}F_{kj} - \delta_{ij}) \text{ where } \delta_{ij} \text{ denotes the Kronecker-symbol} \tag{3}
\]

To get the strain field, the above described procedure was performed for a lot of overlapping cubes which were distributed on a regular grid inside the tomogram of the undeformed state. According to equations (4) and (5), the deformation gradient \( F \) can be decomposed multiplicatively to get the rigid body rotation \( R \) of the cubes.

\[
F = R \cdot U \tag{4}
\]

\[
U = \sqrt{F^T \cdot F} \tag{5}
\]

The displacement vectors were only calculated for such cubes located at the boundary of the region modelled by finite elements. As the number of these vectors (one vector for the center of each cube) was much less than the number of nodal points at the model boundary, missing vectors had to be calculated by interpolation.
4.3. FE-model
4.3.1. Discretization of microstructure
Several requirements concerning an FE-mesh can be formulated: Firstly, the number of FE-elements must be limited in order to achieve acceptable simulation times. Secondly, the phase boundary should be smooth enough to avoid singularities and numerical errors during the FE-simulations, although, real facets of the particles have to be modelled, too. Thirdly, very acute and obtuse angles in the meshes between edges or faces should be avoided which would be accompanied with a disproportion of the edge lengths, since inappropriate angles would also lead to numerical errors.

In principle, a lot of alternative methods exist to convert a voxelized data set (tomogram) to a vectorized mesh, thus to obtain geometric models from tomograms. One possible way is to interpret each voxel as a brick element but this would yield too many elements.

For this reason, in this work the triangles of surface nets indicating the particle/matrix interfaces were used as seed faces for the 3D mesh generation in which a sub-volume is filled by tetrahedra without gaps.

The Marching-Cubes (MC) algorithm was used to build up the surface net.\(^{17}\) With a global threshold and the standard MC-routine of the VTK-library this was performed.\(^{18}\) However, the number of triangles in the surface net was still too high. Therefore, a topology-preserving decimation of the net was done using edge contraction. During this iterative process an error measure was computed and held in memory.\(^{19}\) This measure is used to assign a ”cost” to every possible edge contraction. One of its additive terms measures the geometric accuracy of the net after the contraction, the other accounts for the shapes of the emerging triangles.

The contraction with the least-costs was performed and costs which were influenced by this operation were updated. These steps were repeated until the desired number of triangles was achieved.

Since the triangles in surface serve as seed faces for the tetrahedra mesh generation, the triangle shapes had to be improved further. This was accomplished by a two stage process:

Firstly, the connectivity of the surface net was modified by applying an edge flipping procedure. This procedure aims at improving the regularity of the mesh. In a regular mesh, every vertex has six neighbors, which allows all incident angles to be close to 60\(^\circ\) (which is the interior angle of an equilateral triangle).

Finally, the surface mesh was smoothed by moving the triangle vertices (without changing the connectivity of the mesh). The new positions of the vertices should yield neighboring angles to be fairly equal (i.e. approximately 60 degrees for a vertex with six neighbors) while preserving the geometric accuracy of the surface.

The outcome of the above described procedure is illustrated in Fig. 3. In Figure 3a) an MC net is rendered which approximates the surface of a diamond with 52,308 triangles. After the decimation, edge flipping and smoothing (cf. Fig. 3b) ) the number of triangles is reduced as can be seen when comparing both subfigures. The decimated net contains only 5,000 triangles. Moreover, one can see at a glance that the shape of the triangles in Fig. 3b) is quite equilateral.

Starting from the surface nets of the interfaces between the phases the pre- and postprocessor software MSC/PATRAN\(^{20}\) outputs a 3D FE-mesh automatically when using the so-called TET-mesher which does not exhibit gaps in space. To each of the tetrahedra a phase with its mechanical properties is assigned. Together with the displacement vectors acting upon the surface of the mesh the FE-model is constituted.

In Fig. 4 a typical tetrahedra mesh is shown. The mesh is cut at an arbitrary plane to view inside the mesh. The Co-tetrahedra which intersected by the plane and the tetrahedra representing the diamond (green) are rendered. At a glance it can be seen that the tetrahedra are smaller in the neighborhood of the particle/matrix interface than in the bulk of the material.

In [14] a different path to model real microstructures in 3D was followed. The idea of the voxel-based meshing ibidem was to represent several voxels by one hexahedron element. The density of the FE mesh can be controlled by a voxel binning parameter.

To investigate the influence of element type, the above described meshing meshing with tetrahedral elements was applied to the particle reinforced metal matrix composite (MMC) Al/10vol.%TiN, which was already modelled in [14] by hexahedral elements. In contrast to the hexahedra mesh with its 274,626 elements in [14], the tetrahedra mesh requires only 147,362 elements.
4.3.2. Material properties of phases and simulation issues

The diamond phase in the composite was simulated linear-elastically utilizing the material parameters compiled in table 1. An elastic-plastic behavior given by the hardening curve in Fig. 6 is used for the Co matrix during the FE-simulation. The 3D FE-mesh is comprised of 84,457 tetrahedra. To each tetrahedron of this mesh a phase with its mechanical properties is assigned.

For the current FE-calculations, the modified 10-node tetrahedron of ABAQUS is used. This type of element has three extra internal degrees of freedom (corresponding to an internal node) and are more robust during finite deformation as the standard tetrahedron element. In both cases (hexahedron and tetrahedron), a geometrical and physical nonlinear static finite element analysis was carried out with the large-strain FE-code ABAQUS.

Figure 3. Phase boundary/interface between the Co matrix and a diamond rendered with a) 52,308 triangles and b) 5,000 triangles.

Figure 4. Representation of a cut tetrahedra mesh.

Figure 5. Displacement vectors acting upon the boundaries of microstructural ROI of the Al/TiN composite.
4.3.3. Displacements at model boundaries

The displacement vectors were calculated for the cubes located at the boundaries of the region-of-interest as described in section 4.2. In Fig. 5 the vectors for Al/TiN composite are indicated by arrows whose lengths code the magnitudes of the vectors. In this Figure only the central TiN-particle is rendered. For every node lying on the model boundary a displacement vector had to interpolated from the given vectors. A material extension in loading direction ($z$) and a smaller transverse contraction is reflected by the displacement field depicted in this Figure. The phase distribution, the mechanical properties of the phases and the displacement vectors at the model boundary constitute the FE-model.

5. RESULTS OF DATA ANALYSIS

5.1. Change of particle distances

The relative distance of all particle pairs were computed in such a way that particles lying in almost the same $z$-plane (which is given by a threshold value for the difference of $z$-coordinates) and particle pairs with a minimum distance in $z$-direction were evaluated because of the fact that the $z$-axis is almost parallel aligned to the global loading direction.

From the histograms in Fig. 7 it can be deduced that the specimen elongates in loading direction ($z$) and contracts perpendicular to this direction since the positions of the curve maxima are on the one hand (cf. Fig. 7a) above the zero level and on the other hand (see Fig. 7b) below the zero level.

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**Figure 6.** Hardening curve of the Cobalt matrix computed by a Voce-type equation.

**Figure 7.** Histograms of the relative particle distance changes for particle pairs a) with a minimum distance of 150 $z$-slices, b) with a difference in the $z$-coordinate below 10.
5.2. Strain field

In Fig. 8, the distribution of equivalent plastic strain $\varepsilon_{\text{equ}}$ is color-coded for different $yz$-planes and overlaid over the corresponding 2D CT slices. By this illustration it can easily be recognized that elevated equivalent strains can be found in the neighborhood of the diamonds (cf. Fig. 8b-f). In the technique described in section 4.2 the cube size must be adapted to the characteristic microstructural length given by the mean distance of WC particles. For this reason, a higher strain level is found in the upper diamond 1 (cf. Fig. 8a) but a bluish region in the center of this diamond can also be observed.

![Contour plot of equivalent plastic strain $\varepsilon_{\text{equ}}$ superimposed on different 2D CT slices through the tomogram given by the $x$-indices.](image)

5.3. Comparison of experimental and simulated results

From the sub-volume of the tomogram a region-of-interest was extracted which contained $81 \times 97 \times 105$ voxels. After the 3D FE-simulation of this ROI utilizing the provided displacement vectors the distribution of equivalent plastic strain in an $xz$-plane ($y = 152$) was compared (cf. Fig. 9) with the findings of the strain analysis method described in 4.2. In both color-coded distributions of strain elevated values of strain can be found close to the diamond which is outlined by a magenta polyline. However, the magnitude of equivalent strains differ.

5.4. Effect of the geometric model on the FE-simulation

Fig. 10 shows the maximum principal plastic strain for both modelling procedures (a) hexahedra mesh, b) tetrahedra mesh) in the central $xz$-plane of the MMC Al/TiN. Since the particles are modelled to behave purely elastic, plastic strains can only be developed in the ductile matrix material. In both cases, the images reveal, that the plastic deformation is confined to lumps and narrow bands of high strain. Generally speaking, the contour plots, using a tetrahedra mesh, are more smooth as compared to the hexahedra mesh. The patterns of plastic strain bands agree, however, quite well.

In Fig. 11, the maximum principal tensile stress distribution is shown for both mesh approaches (a) hexahedron mesh, b) tetrahedra mesh). Both contour plots show a location of significant stress concentration at the surface of the center particle. This location corresponds to the position of the experimentally observed cracking of this particle (cf. [14]). In the case of the tetrahedra mesh (Fig. 11b) the stress concentration is less pronounced. In spite of a smaller number of tetrahedral finite elements and less computation time the strain and stress fields are less discontinuous compared to the hexahedron-based modelling. Moreover, the FE-simulations are numerically more stable.
**6. DISCUSSION AND CONCLUSIONS**

In this work the rearrangement and deformation of microstructure of the Cobalt/Diamond composite was imaged by computer tomography. It was shown that even from tomograms obtained by a micro-focus tube equipped CT-scanner strain below 1% can be measured. For the quantification of local displacements and strains two methods were applied:

In the first method 3D data processing operations are executed to identify and characterize individual particles in tomograms which reveal the microstructure in different deformation stages. From the particle mass centers the relative change of particle distances due to macroscopic tensile loading was computed. In a plane perpendicular to that direction predominantly a negative variation of the relative distance change was found. A positive change of the distance was detected in the direction of the tensile force. With the described method the particle distances can be measured with sub-voxel accuracy. In future work a gray value weighted determination of the center of gravity of the particles will be performed to improve the exactness of this method further.

The second method is not dependent on single particle identification since gray level gradients in the sampling
cubes are exploited. The minimum dimension of these cubes is determined by the average spacing between microstructural objects: The edge length of the cube must be larger than this spacing. For each cube the strain tensor was calculated providing a discrete 3D distribution of strain values. Additionally, the displacement vectors at the surface of the sub-volume were computed which were fed into 3D FE-simulations as boundary conditions.

On a real microstructure discretization, three-dimensional nonlinear FE-simulations with boundary conditions interpolated from the above mentioned displacement vectors were carried out. Elevated plastic strains were predicted in the neighborhood of the dispersed brittle phase which could also be found in the measured strain fields.

When comparing the findings of FE-simulations of the MMC Al/TiN with two different finite element types it turned out that the strain pattern are very similar and also a spot of high stress on the particle surface could be found in both simulation results. However, the FE-simulation with the tetrahedron mesh is firstly numerically more stable than the one with the hexahedron mesh due to smoother interfaces between the phases and secondly the number of finite elements (and therefore nodal points) are smaller which reduces computation time. Thirdly, the calculated fields of stress and strain are less discontinuous.

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