

# PROCEEDINGS

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ICDM 1

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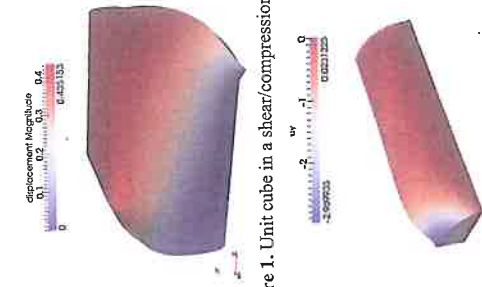


Figure 1. Unit cube in a shear/compression test.

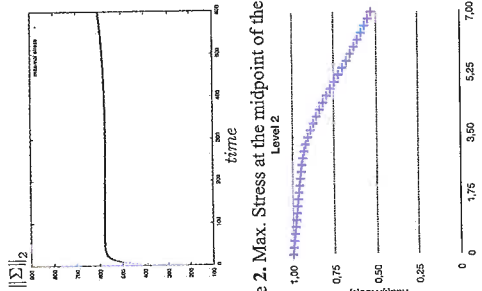


Figure 2. Max. Stress at the midpoint of the cube.

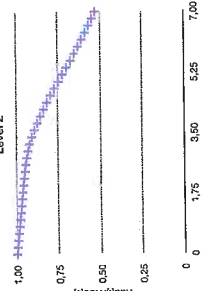


Figure 4. Change of necking area in time

#### 4.2. Software framework UG

UG ([1][8]) is a general-purpose library for the solution of partial differential equations, which supports parallel adaptive multigrid-methods on high-performance computers. A novel implementation ensures the complete independence of grid and algebra. Cache aware storage for algebra structures and a parallel communication layer make UG4 well suited for current and next hardware-architectures.

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## MODELLING OF OVERALL MATERIAL PROPERTIES AND CRACK REINFORCEMENT BY BRIDGING FIBRES IN METAL-CERAMIC COMPOSITES WITH INTERPENETRATING PHASE MICROSTRUCTURE

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**Abstract.** The objective of this paper is the analytical and numerical modelling of the overall elastic properties and the crack bridging toughening mechanism in metal-ceramic composites with interpenetrating phase microstructure (IPC). The specific microstructure of the IPC makes the effective media/field models based on Eshelby's solution inapplicable to the estimation of the effective elastic properties of the IPC. The effective material constants were calculated analytically extending the Tuchinski-Feng models devised for the IPC microstructure. Numerical FEM models were developed for two types of IPC microstructure: simplified 3-D cross structure and real microstructure obtained with computer micro-tomography scans. The micro-CT scans were transformed into FEM meshes using the Simpleware ScanIP/FE commercial software. The crack bridging mechanism was investigated assuming the metal ligament undergoing large plastic deformations (necking) and delamination from the surrounding elastic material (ceramic matrix). As a first step towards the numerical determination of  $J$  integral from the simulation of the CT (compact tension) test, the  $\sigma$ - $u$  relationship in the metal fiber was determined numerically and applied to compute the stress and displacement fields in the CT specimen. The numerical solution agrees well with the analytical one obtained by Mataga et al. [4].

#### 1. Introduction

The metal-ceramic interpenetrating phase composites (IPC) are usually processed by pressure assisted or pressureless infiltration of molten metals into porous ceramic preforms. They have characteristic microstructure different from typical MMC's or CMC's with particulate or fiber reinforcement. The main difference is that both metal and ceramic phases are spatially continuous forming complementary 3D skeletons of non-zero stiffness. The uniform microstructure and the enhanced mechanical and thermal properties are the main advantages of IPC. A state-of-the-art in fracture and damage modelling of IPC can be found in [1], while models of effective properties of the IPC in [2] and [3]. The objective of this paper is twofold: (i) to model the effective elastic properties of IPC, and (ii) to model the fracture in IPC with the crack bridging being the major toughening mechanism. The developed models are verified on the example of  $Al_2O_3$ -Cu infiltrated composites.

## 2. Modelling of overall elastic properties

The effective elastic constants of IPC can be determined using a number of different methods. Firstly, simple estimates of Voigt, Reuss and Hashin-Shtrikman were computed. Secondly, analytical models of Tuchinskii and Feng [2] based on the cross unit cell (Fig. 1) were implemented since the models based on the Eshelby solution are inapplicable for IPC. Here the generic Tuchinskii's model was corrected and extended (cf. curves denoted as "extended bounds" and "extended model" in Fig. 3). Thirdly, numerical methods accounting for a real composite microstructure were developed and used for  $\text{Al}_2\text{O}_3\text{-Cu}$  microstructure acquired from the computer micro-tomography (micro-CT) images (Fig. 2a). The following numerical approaches were compared: the 3D cross microstructure model (Fig. 1), and two models based on the real microstructure obtained from the micro-CT scans: a voxel model, and a model with smoothed interfaces obtained with Simpleware ScanIP/FE software. With the +ScanFE software a FEM mesh was created and a smoothing of the material interfaces and optimization of the size of the elements was done (Fig. 2b). Three effective elastic constants were modelled: Young's modulus (Fig. 3), Poisson's ratio and the shear modulus (here only  $E$  modulus is shown for brevity).



Figure 1. Cross model of interpenetrating microstructure of an IPC.

Figure 2. Real microstructure of  $\text{Al}_2\text{O}_3\text{-Cu}$  IPC from micro-CT images (metal phase) (a), FE representation in ABAQUS via Simpleware ScanIP/ScanFE (b).

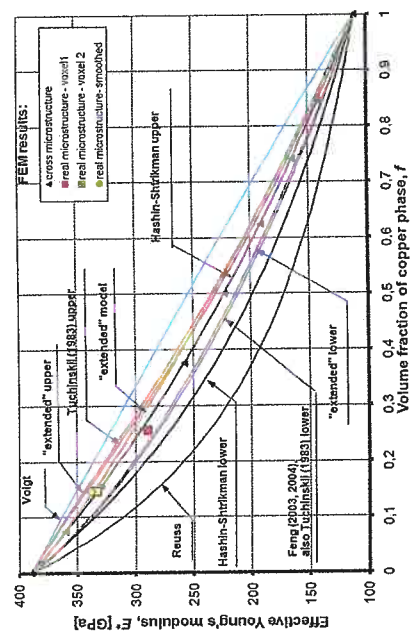


Figure 3. Effective Young's modulus of  $\text{Al}_2\text{O}_3\text{-Cu}$  IPC: analytical and numerical models and micro-CT measurements results.

## 3. Modelling of crack reinforcement by bridging fibres

One of the main toughening effects occurring in metal-ceramic IPC during fracture is the crack bridging by metal ligaments, [4]. These ligaments deform plastically contributing to the composite's fracture toughness. The  $J$ -integral, or energy release rate  $G$  in this case, can be expressed as

$$J = G = \int_0^{u^*} \sigma(u) du \quad (1)$$

where  $\sigma$  is the nominal stress in the bridging ligament at stretch  $u$  ( $\sigma \rightarrow 0$  at  $u = u^*$ , with  $u^*$  being the crack opening displacement COD at rupture). A non-trivial problem is to determine the physical relation  $\sigma(u)$ . This problem was solved numerically in this paper using the model of an elasto-plastic cylindrical ligament in an elastic matrix undergoing delamination from the surrounding material and large strains due to necking. Fig. 4 shows an exemplary FEM solution of axial stress distribution in the ligament for a chosen value of delamination parameter  $\psi$ . The obtained  $\sigma(u)$  relationships in function of the delamination parameter  $\psi$  are presented in Fig. 5 together with the corresponding analytical solutions of Mataga [4] based on purely geometrical considerations.

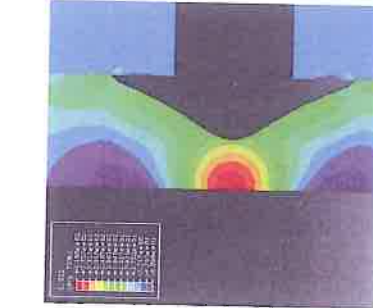


Figure 4. Axial stress distribution in the metal ligament at large plastic deformation and delamination from the matrix; numerical solution by ABAQUS.

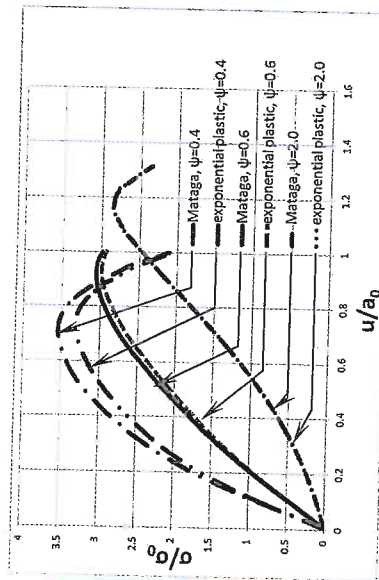


Figure 5. Normalized  $(\sigma-u)$  relationships in metal ligament derived numerically by FEM for three delamination parameters  $\psi$ ;  $\sigma$  and  $\sigma_0$  denote the nominal and the yield stress of the ligament material (Cu);  $a_0$  is the ligament's initial radius. Relevant analytical solutions by Mataga [4] are also shown for comparison.

Having determined the stress-displacement relationship in the bridging fibre, it was possible to apply it as a material model for the fibre in the numerical simulation of the Compact-Tension test. The truss element was introduced similarly as in Emmel [5] to model the bridging of the crack faces. The matrix material of the composite was  $\text{Al}_2\text{O}_3$  ceramics and the ductile fiber was that of copper. The matrix behaviour of the fibre was modelled using the input data furnished by the constitutive relation  $\sigma(u)$  (Fig. 5) which were then used in the UMAT procedure in ABAQUS. The truss element T2D2 was chosen for the fibre. The FEM mesh with boundary conditions and force loading is presented in Fig. 6.

An illustrative example of the computed stress field in the CT specimen with a single metal ligament bridging the crack faces is shown in Fig. 7.



**Figure 6.** The FEM mesh of a CT specimen with the metal ligament modelled as truss element connecting the crack faces.

**Figure 7.** Vertical stress distribution (numerical solution by ABAQUS)

#### 4. Conclusions

A set of analytical estimates and numerical models have been employed to determine the effective elastic constants of the interpenetrating phase composites. The micro-CT images have been incorporated in the developed FEM models leading to the most realistic estimates of elastic constants. A problem of crack bridging with ligament undergoing delamination and necking has been modelled by FEM for an idealized ligament geometry. The resulting  $\sigma$ - $u$  relationship for the crack bridging fibre was used in the FEM model of the Compact-Tension test. The obtained numerical results enable calculation of the  $J$  integral which is now in progress.

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## MULTISCALE MODELING OF COLLECTIVE BEHAVIOR OF CARBON NANOTUBES

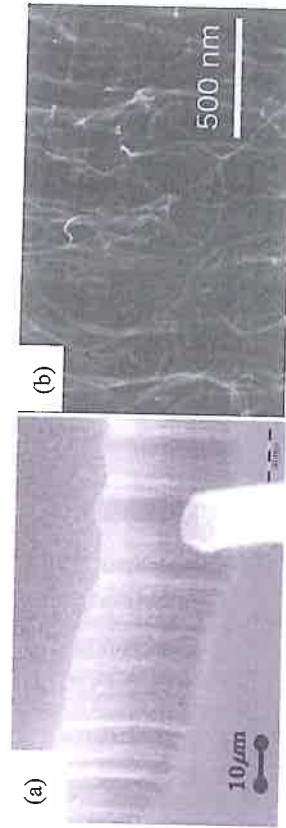
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**Abstract.** To analyze the collective behavior of a large number of carbon nanotubes (CNTs) we consider two computational models, covering two different length and time scales. To model a large number of interacting CNTs in a turf, we represent the segments of CNTs forming the turf, as elastica finite elements. During compression, the predominant deformation of CNTs is due to bending and buckling. The van der Waals forces of interaction between adjacent tubes are modeled as distributed loads. An explicit time integration technique is used to integrate the equations of motion. The resulting computational model is robust and is capable of modeling the collective behavior of CNTs. The generation of the computational model of a turf is accomplished by means of the restricted random walk and subsequent relaxation. The continuum model is a nonlinear viscoelastic model. We show that it is capable of representing different experimental conditions.

#### 1. Introduction

The properties of individual carbon nanotubes (CNTs) have been studied extensively, and are now well understood. The collective behavior of CNTs arranged in complex structures, *turfs* (Figure 1) is of interest in practical applications, such as nanoscale sensors and thermal switches. Their microstructure is the result of the growth process from the substrate [1], during which an interplay of elastic bending energy and adhesive energy produces a local energy minimum in the configurational space [2].



**Figure 1.** SEM images of the carbon nanotube turf: (a) corner view, (b) detail.

Given the growth method, the following question arises: Is the CNT turf a *material*, describable by a standard mathematical apparatus of continuum mechanics with effective properties, or – is it a *structure*, in which case a continuum model is not relevant?