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NUMERICAL MODELING OF FRACTURE TOUGHNESS OF METAL-CERAMIC INTERPENETRATING PHASE COMPOSITES WITH ACCOUNT OF MATERIAL MICROSTRUCTURE

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Introduction

The motivation for research on interpenetrating phase composites and possible applications of these novel materials were given in [1]. A rationale behind designing an IPC is to achieve a highly durable material that would combine the most desirable properties of the constituent phases: the high hardness and wear resistance of ceramic and improved fracture toughness and thermal conductivity due to the metal content. The interpenetrating metal-ceramic composites may have remarkable applicability in different sectors of industry, e.g. automotive and aerospace. They should, thus, be carefully investigated in terms of processing routes, material properties and modeling of material response to service conditions.

A 3D FEM model in ABAQUS of the fracture parameters and crack growth in bi-continuous metal-ceramic composites with interpenetrating microstructure (IPC) is proposed. The crack is modeled using the extended finite element method (XFEM) [4]. The *J*-integral and fracture toughness K_{Ic} are determined for a real IPC microstructure obtained from micro-CT images. The fracture parameters (i.e. fracture toughness K_{Ic}, *J* integral, crack opening displacement) are key mechanical characteristics of IPC composites because of the brittleness of the ceramic phase. The main effects occurring in metal-ceramic IPC during fracture are described (cf. [2], [3]).

Modeling of fracture toughness K_{Ic} of metal-ceramic IPC

The real IPC microstructure obtained via computed microtomography (micro-CT) (Fig.1c) was incorporated in the present model to give the most accurate microstructure representation. The microstructure images obtained with micro-CT were transformed into a finite element mesh using Simpleware ScanIP/FE software. A scheme of the Compact-Tension (C-T) test model (Fig. 1b) created with ABAQUS for a copper-alumina IPC with the real microstructure in the vicinity of the crack, is depicted in Fig. 1. The effective properties of the composite without a crack were obtained with earlier developed analytical models [5] (Fig. 1a). The IPC microstructure was introduced into the model of the C-T specimen in front of the crack tip. The alumina preform was modeled as isotropic elastic, while the copper infiltrating phase as isotropic elasto-plastic with isotropic hardening.

730322 (outer part) + 216000 (real material part) solid C3D8 finite elements were used in computations. Large strains locally occurring in the metal ligament necking zone were determined by an incremental algorithm. The surface interaction between copper and ceramic was modeled as cohesive, using the results of [6]. Since large microstructure data was involved, only a small volume near the vicinity of the crack tip was modeled using the micro-CT scans, with the remaining part taken as an effective elastic medium. Submodeling was used to combine the calculations for both subdomains of the specimen, with results from the outer part transferred onto the real material part through the layer of common nodes. Moreover, only a slice of the CT specimen of approx. 0.5mm thickness was considered in the ABAQUS calculations. A displacement-controlled quasi-static loading was applied to make the crack growing.

$$\dot{\varepsilon}^v = \frac{\boldsymbol{\sigma}'}{2\eta_s} + \frac{\mathrm{tr}(\boldsymbol{\sigma}) - 3\sigma_s}{9\eta_b}\mathbf{I} \tag{1}$$

where $\boldsymbol{\sigma}'$ is the deviatoric stress, $\mathrm{tr}(\boldsymbol{\sigma})$ – the trace of the stress tensor, σ_s – the sintering stress, η_s – the shear viscosity modulus η_s – the bulk viscosity modulus.

In the multiscale approach, macroscopic constitutive properties, including the elastic moduli, bulk and shear viscosity, as well as the sintering driving stress are determined from micromechanical simulations of sintering. The micromechanical model of sintering has been developed within a framework of the discrete element method [2]. The DEM considers large assemblies of particles which interact with one another through contact forces. The rheological scheme of the contact model for sintering is shown in Fig. 1b. It includes elasticity, thermal expansion, viscosity (creep) and the sintering driving force, which is consistent with the macroscopic model.

The constitutive parameters of the DEM model of sintering depend on the parameters which can be determined using atomistic models. The methods of molecular statics and dynamics will be used to determine the elastic constants, surface energy and diffusion coefficients used as input data in microscopic sintering models.

4. Case study

Sintering of NiAl powder has been analysed as a case study using the multscale approach. Figure 2 shows selected mechanisms of diffusion considered in the molecular statics analysis. Average shear viscous modulus determined from the DEM simulations is plotted in Fig. 3 as functions of sintering time and relative density.

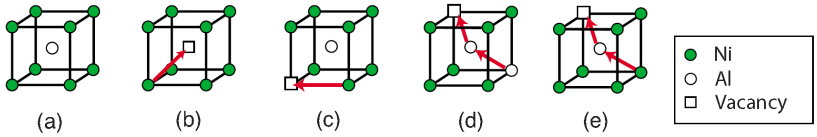

Figure 2. Schematic representation of NiAl crystal structure and selected hop mechanisms [3]

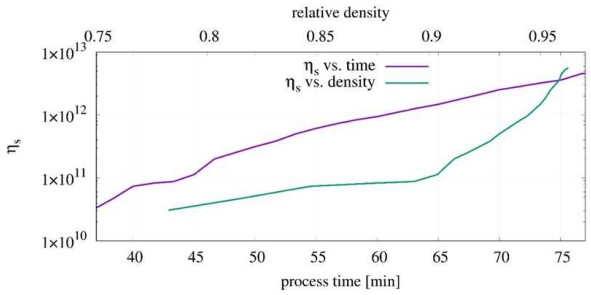

Figure 3. Average shear viscous modulus determined from the DEM simulations

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5. References

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