Process Simulation and Prediction of Fracture Probability in Powder Technology

The Institute for Materials Applications (IWM)/DE and the Institute for Applied Powder Metallurgy and Ceramics (IAPK)/DE at the RWTH Aachen e. V./DE work on a "powder-to-product" framework based on numerical simulation. Today, the framework encompasses important steps of the process chain for Powder Metallurgy (PM) and ceramic products including powder filling, sintering, HIP, and lifetime prediction. The present article highlights three examples of successful integration of simulation tools along the powder-technological production chain.

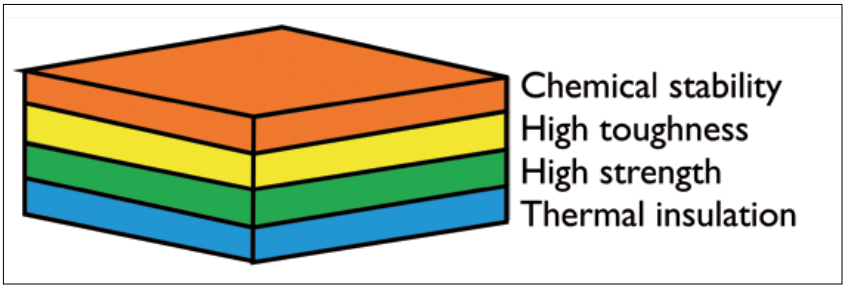

Fig.1
Example property profile of an MLC

Introduction

Ceramic materials feature several excellent properties such as chemical resistance, thermal stability, and high compressive strength. However, their use as structural components is severely limited by their susceptibility to failure under tensile stress, their statistically distributed strength, and their low fracture toughness. Multilayer Laminated Ceramics (MLCs) offer attractive capabilities to mitigate this drawback as combinations of weak and strong layers, as well as weak or strong interfaces can be used to improve an MLC's apparent fracture toughness through the introduction of crack deterring mechanisms. Additionally, the materials and material grades used in a laminate can be tailored to the prospective application, yielding a property profile that situates the best suitable materials at the location where they are needed most (Fig. 1).

It is well known, that the properties of ceramic components depend significantly on the manufacturing process with which they are made. In structural ceramics, major challenges in manufacturing are to achieve a final component shape that requires a minimum amount of post-processing (due to high tooling costs) and to realize the desired mechanical stability. The latter challenge is due to the inherent brittleness of ceramics especially important for components that are loaded under tensile stress. The driving factor for tensile failure of ceramics is the distribution and size of flaws or discontinuities in the material. These include amongst other pores, foreign matter inclusions, undesired density gradients, surface roughness, and material interfaces. Because most, if not all, of the flaws are introduced by the particular processing methods, it is important to consider the whole production process and its influence on the final product's properties when designing a ceramic component.

Before the introduction of simulation tools, the design of near-net-shape and defect free components required a costly trial-and-error approach. In recent times, however, shorter computational times have led to the development of computational models for process simulation that can be applied at different scales and for different processing stages. The Institute for Materi-

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als Applications (IWM) and the Institute for Applied Powder Metallurgy and Ceramics at the RWTH Aachen e.V. (IAPK) work on a "powder-to-product" framework based on numerical simulation. Today, the framework encompasses important steps of the process chain for Powder Metallurgy (PM) and ceramic products including powder filling, sintering, HIP, and lifetime prediction. The present article highlights three examples of successful integration of simulation tools along the powder-technological production chain. In the initial stage of the production, the influence of green density on the sintering behaviour is evaluated for die filling. Subsequently, the use of Finite Element (FE) tools to predict the deformation and residual stress behaviour of co-sintered ceramic laminated composites is elucidated by means of a bilayer ceramic laminate. In the last stage, the method for predicting the fracture probability and lifetime of sintered components is elaborated. The aim of these modelling methods described in this article is to showcase the design tools for ceramic components, which allow predictions of the final shape, residual stresses, and the reliability of the final product, in the stage of the ceramic design process. This reduces the need for the often-costly prototypes and trial-and-error processes that are nowadays inherent to the design of structural ceramic components.

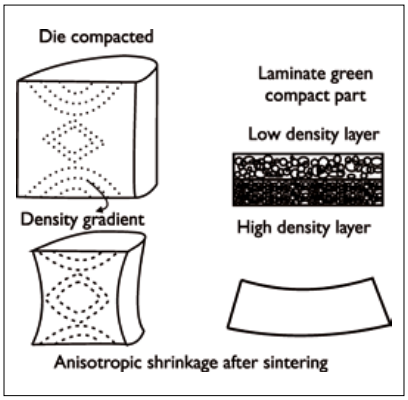

Fig. 2
Influences of the density gradients on the final sintering component

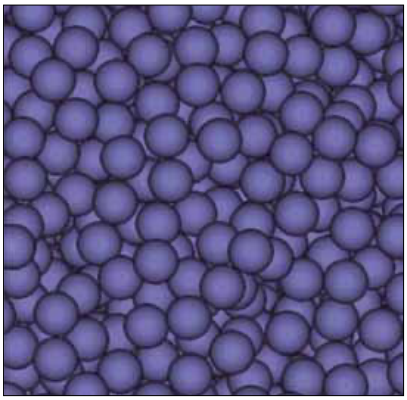

Fig. 3
An example of three-dimensional mono-sized sphere filling

Simulation of powder filling and green body

Prior to sintering, the shaped ceramic powders are generally referred to as the green body. This can be obtained by means of different filling methods, e.g. axial or isostatic compression, tape casting, injection moulding, and also with new 3D-printing technologies such as binder jetting or lithography. The density of the green body is increased by compaction or drying during green body production, which often introduces density gradients. During sintering, dense regions sinter at higher rates than sparse regions, which causes shape distortion and residual stresses that may lead to premature component failure. The study of the influence of the initial density distribution on the final shape of sintered components is one of the most essential aspects in recent powder-filling models. Two examples are shown in Fig. 2, the density gradients in the die compacted material result in anisotropic shrinkage and a distorted final shape [1].

To generate the initial green density distribution, a methodology to determine the relative density distribution (or powder packing) through Image Analysis (IA) was developed [2]. The experimental results were used to develop a powder-filling model based on the Discrete Element Method (DEM).

DEM is a particle method based on Newton's laws of motion. Particles can move with six degrees of freedom (three for translational and three for rotational movement). The particles are defined as soft-particles with consideration of material deformation. During the calculation, a contact model is applied to calculate the contact forces between individual particles. Furthermore, external forces such as gravity or external pressure can be introduced into the simulation as well. An example of a three-dimensional mono-sized sphere filling is shown in Fig. 3.

With the consideration of different factors such as material properties, interparticle friction, and particle size, these mono-sized particles fill approximately 59 – 63 % of the die's volume. Therefore, the particle size distribution can be implemented in the simulation. Subsequently, the effects of vibration and compaction on the filled die can be simulated, by which the segregation and the corresponding density gradient are determined.

A DEM simulation is divided into three different steps (Fig. 4) [3]: model design by pre-processing, simulation and solution by numerical simulation, export and evaluation by post-processing. After the DEM

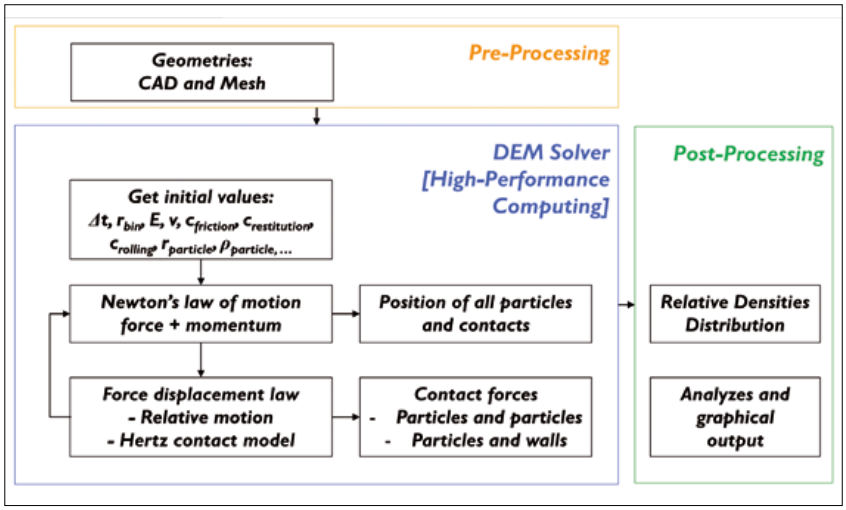

Fig. 4
DEM modelling approach for determination of initial density distribution

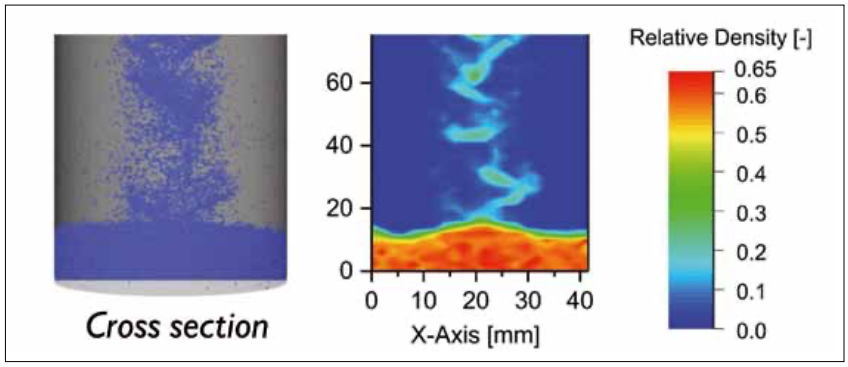

Fig. 5
An example of die filling on cross section and the powder density distribution with monosize powder

simulation, the positions of the particles, the contact forces between particles, and the contact forces between the particles and the die are included in the output data. Using in-house scripts, the relative density distribution (Fig. 5) is calculated and exported to a sintering model, in which the next processing step may be simulated.
The DEM model is well equipped to simulate particle filling and packing and thereby allows for the prediction of possible unwanted density gradients when selecting the green body processing method for a newly designed component. The effect of inhomogeneous density distributions on the deformation behaviour can be simulated with a compaction sintering model, which was implemented in in-house developed user subroutines for the finite element (FE) software ABAQUS [4]. In this way, the anisotropic deformation can be accurately predicted by numerical simulations.

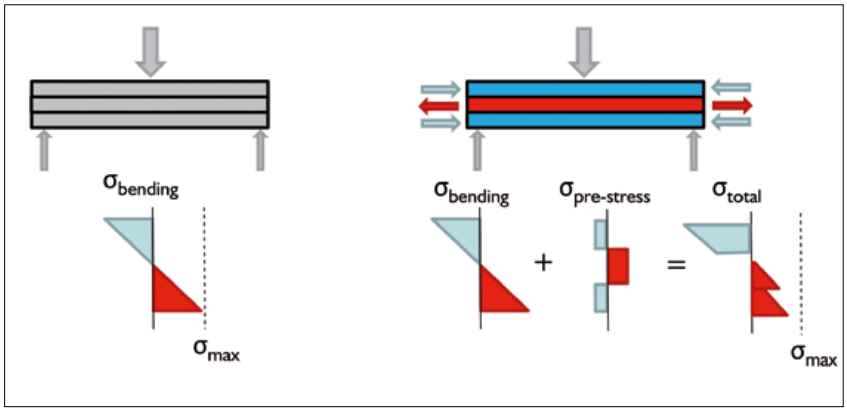

Fig. 6
Influence of pre-stress on maximum tensile stress in 3-point-bending of MLC bars

Fig. 7
Evolution of a bilayer ceramic during co-sintering (f. l. t. r.)

Simulation of sintering

MLCs are often manufactured using the co-sintering process in which individual, tape cast layers are laminated in the green state before being sintered as a green laminate [5]. During co-sintering, each layer experiences sinter shrinkage and thermal expansion. These mechanisms depend on the material's chemical composition, the properties of the used powder (e.g. particle morphology and size distribution), and the process by which the green body is manufactured. The last factor may be responsible for anisotropic shrinkage behaviour as it may cause a bias in particle orientation (e.g. tape casting) or packing density (e.g. uniaxial compression). Combining layers with different sinter shrinkages or thermal expansion coefficients allows for the incorporation of residual stresses (or pre-stresses) (Fig. 6) that can significantly improve the apparent strength and toughness of an MLC. Additionally, by predicting the expected deformation resulting from internal stresses, the green body can be designed such that the necessary shaping during post-processing is minimized. Unfortunately, residual stresses may also lead to undesired deformation and in the worst case, premature component failure (Fig. 7). Therefore, it is of paramount importance to consider the layer compatibility before laminate production.
The considerable amount of available materials and material grades offers the MLC technology an incredible versatility. This, however, is inextricably linked to a highly complex design process that considers the interaction between different materials during co-sintering and results in near net shape and failure-free MLCs. In the laminate design phase, not only the desired component geometry but also the free sinter shrinkage and thermal expansion of individual layers should be attenuated. It follows that a higher strain differential induces higher residual stresses, which may lead to fracture. In addition, the thickness of each layer and its location in the laminate should also be considered. These determine the component's ability to alleviate residual stresses through material relaxation and macroscopic deformation.
The IAPK and IWM have implemented and use viscous sintering models in an FE environment to predict layer densification, component deformation, and resid-

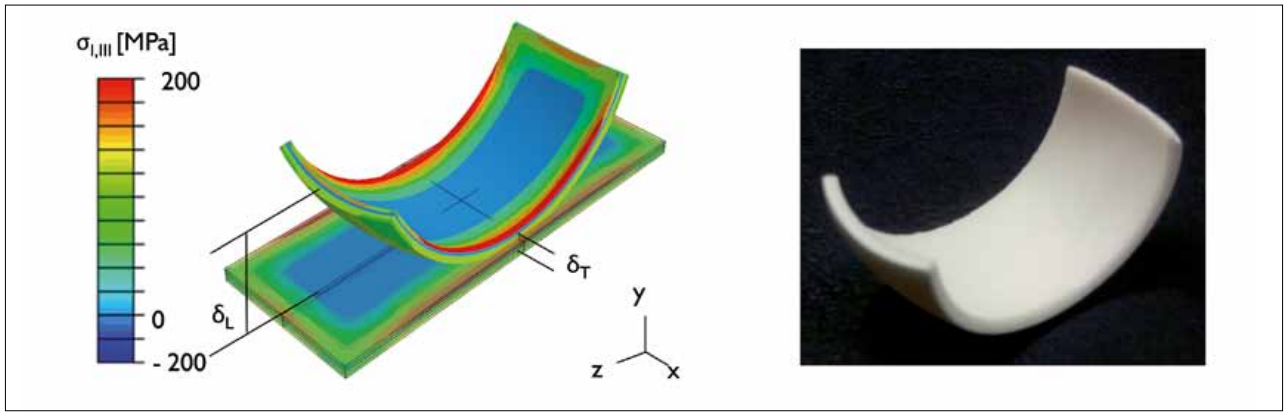

Fig. 8
Simulation of deformation and residual stress (l.) compared with experimental deformation (r.) (samples provided by R. Hammerbacher, A. Roosen, University of Erlangen-Nuremberg/DE)

ual stresses during co-sintering of MLCs (Fig. 8) [6]. Under the assumption of the linearly viscoplastic behaviour, the model's input parameters can be obtained from relatively straightforward viscosimetry (Fig. 9) and (optical) dilatometry experiments.

A combination of the co-sintering models with discretized optimization schemes allows the IAPK determining the optimum laminate configuration for a given application from a pre-existing material portfolio. Ultimately, the simulations yield tailored designs for near-net-shape MLCs with improved strength and toughness for high performance applications.

Simulation of fracture probability and lifetime

Due to the intrinsic structures of ceramics, flaws in ceramic components can be easily induced in nearly every processing step. Therefore, flaws in ceramic products are inevitable. They also often show a large scatter in size, as well as a distribution throughout the component in terms of location and orientation [9]. Flaws generally lead to failure, in which one can distinguish between instantaneous (brittle) fracture induced by exceedance of the component's ultimate load and time dependent failure due to subcritical crack growth, induced by e.g. cycling loads, environmental conditions, or residual stresses in the material. To determine the load limit of ceramic components to avoid failure under tensile loads, the flaw size and distribution must be determined. To define the component's reliability, the time and loading cycle dependent failure mechanisms must be considered. The failure behaviour of ceramics is usually studied with the classical Weibull approach in the frame of statistical fracture mechanics. IAPK and IWM have developed the necessary experimental setups and simulation tools [10]. The previously discussed green body and sintering simulation tools can be used to evaluate the possible influence of component manufacturing on factors af-

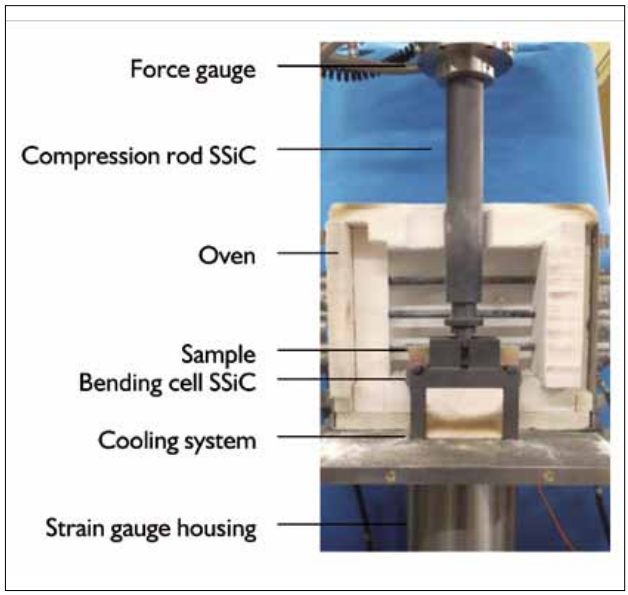

Fig. 9
High-temperature bending and viscosimetry setup

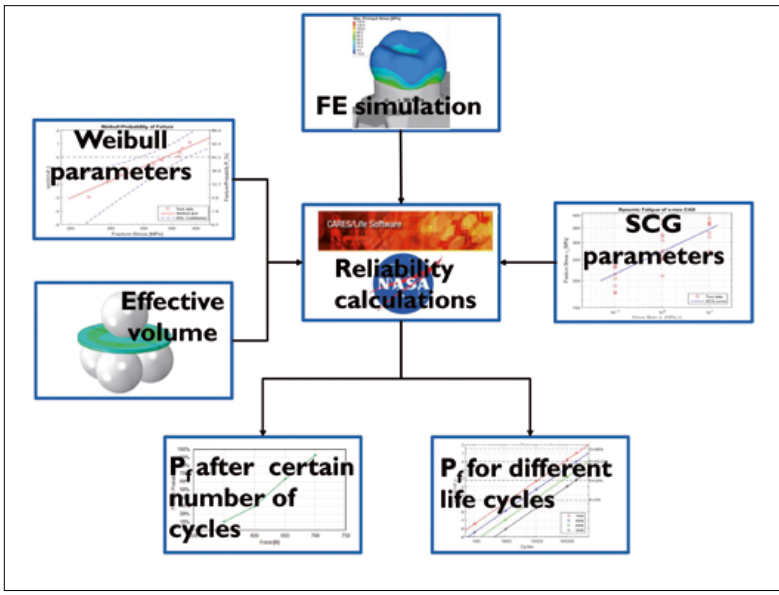

Fig. 10
Prediction of fracture probability of a ceramic component

fecting the limit load and life time. A flow chart for the prediction of fracture probability of a ceramic component is shown in Fig. 10.

Predicting the fracture probability of complex components or components under complex loading conditions requires a combination of strength experiments and simulation tools. The Weibull and slow crack growth (SCG) parameters are determined based on strength tests for samples with a straightforward geometry and well-defined loading conditions. Thereby the two Weibull parameters (Weibull modulus and characteristic strength) can be determined based on the maximum likelihood estimator (MLE) method [7]. The SCG parameters can be obtained based on the linear regression method [8]. Since the Weibull parameters are not only material but also geometry and process dependent, they need to be decoupled to be able to be used for the fracture probability prediction of differently shaped components. This requires the use of the Weibull size effect, which shows how the experimental parameters determined for a particular geometry and loading condition can be transformed to other geometries and loading conditions if the effective volume of the initial test case is known. The effective volume is a measure for the distribution and severity of tensile stresses in a component or sample. Depending on the type of test, the effective volume can be calculated analytically or numerically. For uniaxial tests such as the 4-point bending (4PB) test or 3-point bending (3PB) test, the effective volume can be obtained directly based on the corresponding analytical solutions [7]. However, for the ball-on-3-ball (B3B) test or pin-on-disk test, which are biaxial tests, analytical solutions do not suffice. In this case, FE-simulations should be used to calculate the effective volume. After the effective volume is obtained, the corresponding Weibull scale parameter can be calculated. This parameter corresponds to the stress level where 63,2 % of specimens with a unit volume would fracture. Compared to the classical characteristic strength, this parameter holds more significance because it is a material property regardless of different geometries and loading types.

After the determination of the Weibull parameters, a FE-simulation is employed to obtain the maximum principal stress distribution in a complexly shaped ceramic component under application specific loading conditions. For components that contain viscoelastic materials such as glass, the residual stresses play a non-trivial role in the failure behaviour and therefore must be considered. In that case, the residual stress state is determined prior to the fracture probability calculations using the previously discussed sintering models or alternatively, thermomechanical models.For the fracture probability and lifetime prediction, the numerically determined stress distribution and the experimentally determined Weibull and SCG parameters are combined to calculate the fracture probability of the component using the program CARES/LIFE. This is based on the principle of independent action (PIA) or the more sophisticated Batdorf model [11].

A standard approach to evaluate the reliability of complex ceramic components is not yet established in the literature [12]. Many authors [12–16] have concluded that the FE simulation in combination with the post-processor CARES/LIFE represent an optimal approach to predict the load and time dependent fracture probability.

Summary

Different stages of the production process of structural ceramics exemplarily have been simulated in the computational framework established at IAPK and IWM. DEM-simulation can be used to predict density gradients in powder compacts. This allows the user to gain insight in the die filling process prior to production. Using FE-sintering simulation, the densification of powder fillings and compacts under the influence of time, temperature, and external stresses can be predicted. A combination of the DEM- and FE-simulations can thereby be used to establish near-net-shape components, as well as components with tailored residual stress distributions that may be used to reduce peak stresses. Using the simulation results, the influence of the production process through the powder distribution and the induced residual stresses can further on be used to predict the reliability and prospective service lifetime of ceramic components. Here, a combination of statistical methods and the commercial software CARES/LIFE is used.

Designing structural ceramic components is no straightforward matter. Fortunately, nowadays the available computational capabilities and sophisticated software tools allow us to gain insight in the expected behaviour of ceramics during the production process and to predict the final component properties. Thereby, we may save significantly on costly parts of the design process, for example by negating the need for a conventional trial-and-error approach.

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