Journal of the European Ceramic Society 36 (2016) 2245–2253

Contents lists available at www.sciencedirect.com

Journal of the European Ceramic Society

journal homepage: www.elsevier.com/locate/jeurceramsoc

# Discrete element simulation of metal ceramic composite materials with varying metal content

Robert Besler[a], Marcel Rossetti da Silva[a], Maksym Dosta[b], Stefan Heinrich[b], Rolf Janssen[a,*]

[a] Institute of Advanced Ceramics, Hamburg University of Technology, Germany
[b] Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Germany

ARTICLE INFO

*Article history:*
Received 28 October 2015
Received in revised form
30 December 2015
Accepted 31 December 2015
Available online 12 January 2016

*Keywords:*
Discrete element method (DEM)
Sintering
Composites
Metal/ceramic
Alumina

ABSTRACT

Metal–ceramic composite materials are used in several fields of industrial applications. Most of the composites are particulate composites, where metal is the matrix and ceramic the reinforcing particulate material. Oxide dispersion strengthened alloys show increased temperature stability compared to the pure alloy. Theoretical models describing the densification evolution during sintering are only available for particle reinforced materials, but there are no models developed for interpenetrating structures, when both phases are sintering.

We present a modelling approach based on the discrete element method, which can be used to investigate the sintering behavior on the whole range of powder metallurgical producible composites. The discrete element method takes the particulate structure of the powder compact into account and allows one to perform detailed modelling of each contact separately. In this paper the metal fraction was varied between 100 and 0 vol.% and the densification was analyzed by the contact radius evolution.



## 1. Introduction

The sintering process is a key step in ceramic processing, which assigns to the quality of the finished product. The final shape, microstructure and properties, e.g. density and heat conductivity, develop during this stage from a powder compact. The microstructure and densification of the powder compact evolve due to the rearrangement of single particles in the first two stages of sintering and due to the changes in shape and size of them in the last stage. During this process the powder compact undergoes shrinkage and the center of mass of each particle approaches each other. Many factors as temperature gradients, external forces or inhomogeneous density distribution in the green body can influence the development of microstructure, shape changes and densification. Advanced applications demand a specific microstructure and/or density, which are only possible to control if the process of sintering is well understood.

The understanding of the sintering usually requires high effort in empirical analysis. Due to the complexity of this process, the number of needed experiments can rise up and leads to a significant increase of required time and costs. Here, mathematical models can be used to describe a problem well enough to gain understanding and predict the densification and/or microstructure. The most applied sintering models so far use the continuum mechanical approach. This approach was reviewed by Bordia and Scherer [1–3] in the late 80s and by Olevsky [4] in 1998. Recently it has been used to investigate hot isostatic pressing and free sintering by Galuppi and Deseri [5]. To analyse the evolution of micro- and macrostructures an approach based on the Monte Carlo method was also applied by many researchers [6–8]. However, the most promising approach, taking the particulate structure of the material into account, is the discrete element method (DEM[1]) developed by Cundall and Strack [9]. One significant advantage of this method is, that each particle is treated as an individual discrete element with all degrees of freedom. Therefore, the motion of each particle and forces acting on it can be effectively described. Despite the simplified representation of solid particles as ideally spherical objects, the

*Abbreviations:* DEM, discrete element method; NCR, normalized contact radius; T.D., theoretical density; ACN, average coordination number.

* Corresponding author. Institute of Advanced Ceramics, Hamburg University of Technology, 21071 Hamburg, Germany.
*E-mail address:* janssen@tuhh.de (R. Janssen).

[1] Discrete element method.

http://dx.doi.org/10.1016/j.jeurceramsoc.2015.12.051
0955-2219/

DEM results are in good agreement with real processes in process engineering, material handling and material science [10].

Nowadays, the field of new composite materials is a highly developing field of research in the discipline of material science. The manufacturing of composites provides a final product with advanced characteristics. This can be achieved through the combination of several separate materials. Therefore, composites have a wide range of engineering applications from sports' equipment to spacecraft' [11]. Composite materials, especially particle reinforced composites, can be produced by powder metallurgy in an economic way. In this manufacturing process the blend of different powders is compressed and sintered. Still, only few DEM simulations on sintering of composite materials have been done so far [12–14]. All these works consider the reinforcing phase, e.g. ceramic, as rigid inclusions and investigate only particle reinforced composite materials at low particle concentrations («30 vol.%). To cover the whole range of composite materials the assumption, based on rigid inclusions is not valid.

The general purpose of this work is to simulate free solid-state sintering of composite materials at a fixed temperature. The investigated material consists of two phases and the sintering of both materials is simulated using the "in house" made DEM based simulation system MUSEN-DEM [15]. The metal phase is represented with nickel and the ceramic phase with alumina. The densification behavior has been compared for compositions with 100, 90, 80 (metal matrix material), 60, 40 (interpenetrating materials) and 20, 10 and 0 vol.% nickel (ceramic matrix materials). Special emphasis was given to the interactions between the metal and ceramic particles.

## 2. Simulation method and virtual samples

### 2.1. Discrete element method

Several industrial applications as well as many phenomena in nature involve particulate media. The discrete character of the medium results in a complex behavior due to the dynamic interaction between particles and their interaction with the environment [9].

Cundall and Strack developed in 1979 the discrete element method (DEM) to study rock mechanics. This method takes into account the granular nature of the material by treating every grain as a discrete element with all 6 degrees of freedom. The motion of one single particle is described with the sum of all acting forces and moments. These can be forces in normal and tangential direction caused by the contact between particles, pressure gradients, gravity, drag, etc. To describe the motion of particles Newton's equations of motion are iteratively solved for each individual object. Thereby, simulations with the DEM can provide detailed information, such as trajectories, position of individual particles, forces acting on them, etc [16]. It is extremely difficult to obtain such data by experiments.

Despite the high computational effort, nowadays the DEM approach is widely used to investigate various engineering problems. Deen et al. investigated fluidization processes where DEM was coupled with computational fluid dynamics (CFD) [17]. An et al. investigated the vibratory ball milling [18] and Mirsha and Murty did some simulations on a ball milling process [19]. Zhu et al. wrote a review on the applications of DEM [10]. In the last decade the interest to this method was significantly increased in the field of material science, where it was applied to model e.g. the compaction of ceramic powders [20], compression tests [21,22], bending tests [23] and – most relevant here – sintering. Martin et al. investigated the sintering of copper at varying temperatures [24], crack evolution for constrained and unconstrained sintering [25] and the effect of substrate for film sintering [26]. Henrich et al. investigated free and pre-assisted solid-state sintering with special focus on the particle rearrangement [27], stress induced anisotropy through sintering of alumina [28], the effect of particle size distribution on solid-state sintering [29] as well as the influence of initial coordination number [30].

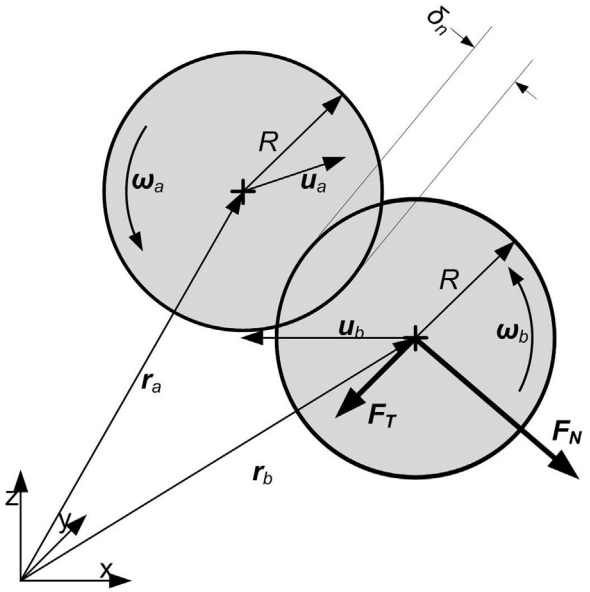


**Fig. 1.** Schematic representation of two particles in contact.

However, only very few investigations have been done on the sintering of composite materials. Jagota and Scherer investigated the sintering of a composite, consisting of three-dimensional randomly packed equal sized spheres [14]. Olmos et al. simulated the sintering of particulate alumina reinforced copper composites and compared the results with experimental data [12]. They observed an interaction between copper and the rigid alumina particles. Yan et al. did a study on the effect of volume fraction, size and packing homogeneity on the sintering behavior of a metal matrix composite with rigid ceramic particles [13]. They simulated the behavior of metal particles with the soft sphere and the ceramic particles with the hard sphere approach at a sintering temperature of 800 °C.

In the previously published works the ceramic phase of composites was treated as rigid inclusions, whereas the metal sinters as monolithic material. As a consequence, only one material sinters and the other follows an elastic law. Therefore, such simplification is only valid for particle reinforced composite materials at low temperatures. In the interpenetrating range, at high temperatures, both materials will sinter and this will be considered in the following chapters.

### 2.2. Modeling concept and generation of modeled structure

To simulate the sintering behavior up to a relative density of 90%, a modified soft sphere contact model has been employed [26]. This model is used to describe the contact force acting between interacting particles with positions $r_a$ and $r_b$, as it is schematically shown in Fig. 1. The force is calculated only between contacting particles, when the overlap $\delta_n > 0$.

As in a previous publication [13], here nickel (Ni) was simulated as the metal material and alumina ($Al_2O_3$) as the ceramic. For the simulation of the composite a special approach was developed, where the following three different types of contacts have been considered: