Powder Technology 248 (2013) 77–83

Contents lists available at ScienceDirect

Powder Technology

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

Three-dimensional discrete element modeling of micromechanical bending tests of ceramic–polymer composite materials ☆

M.F.H. Wolff [a,*], V. Salikov [a], S. Antonyuk [a], S. Heinrich [a], G.A. Schneider [b]

[a] Hamburg University of Technology, Institute of Solids Process Engineering and Particle Technology, Denickestr. 15, 21073 Hamburg, Germany
[b] Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, 21073 Hamburg, Germany

ARTICLE INFO

Available online 20 July 2013

Keywords:
Discrete element method
Mechanical properties
Mechanical tests
Composite material
Packing density

ABSTRACT

Ceramic–polymer composite materials are used throughout materials science, but theoretical models which take into account the microstructural design to predict their mechanical properties are still not fully developed. We present an approach to use the discrete element method to model the mechanical behavior under bending load of dense composite materials made from ceramic particles which are bonded together by polymeric layers. Unlike many other modeling approaches, the internal particulate structure of the material, including the particle size distribution, packing structure, and pore structure can thus be considered. Linear-elastic bonds are created between all contacting particles to model the polymeric binder. A three-dimensional beam with a packing density of 63% is generated and its mechanical properties are tested in 3- and 4-point bending. The loading speed, loading scheme (position of the supports), and the mechanical properties of the polymeric bonds are varied and their effect on the modulus of elasticity of the material is investigated.

1. Introduction

Materials made from ceramic powders are studied and used for applications in materials sciences and industries, ranging from sophisticated machine elements to applications in everyday life, such as tableware made from porcelain. The versatile use of this material class is a consequence of a number of useful properties, including its electrical and mechanical properties, and its abundance in nature. However, the structural applications of ceramic materials are often limited by their high brittleness and scatter of mechanical properties resulting in the lack of predictability of the material failure. Furthermore, for ceramic materials it is very difficult or impossible to tailor their mechanical properties. On the other hand, polymeric materials in general exhibit a number of properties which are more or less complementary to the ones of ceramic materials, such as high ductility, adjustability, but relatively low modulus of elasticity and strength. Naturally, these two materials have been combined for many years to form composite materials.

Unlike in pure ceramics, customized mechanical properties with high strength and high fracture toughness are feasible to obtain by varying the type and amount of the two phases as well as the interface strength on different length scales [1]. To achieve a high modulus of elasticity and hardness of the composite material, it is vital to have a high amount of the ceramic phase in the material and only a small amount of the polymer. Nature has created many of its materials in exactly this way, leading to outstanding filling degrees of up to 95 vol.-% ceramic phase [2]. These materials combine high stiffness, strength, and toughness, and have been studied extensively in recent years [1,3]. Taking them as a role model for engineered materials, there is still a lot of room for improvement in the structural design of filled composite materials.

In order to develop an understanding of the complex mechanisms and structure-property relationships of composite materials, it is necessary to simulate their behavior using advanced models and modeling techniques. The influence of certain parameters under otherwise equal conditions can thus be studied much easier and more reliably than it would be the case if all structures for all parameter variations had to be synthesized and tested experimentally. In particular, it is rather straightforward to study experimentally the modulus of elasticity of polymer composites for small and medium filling degrees, but it is much harder to do the same for high packing densities (>60 vol.-%) and varying properties of the polymer under otherwise unchanged conditions, because the preparation of such samples is tedious, particularly regarding the homogeneity of the samples.

Numerous investigations have been made to study the mechanisms of mechanical reinforcement of polymers, considering the size, shape, and filling degree of the reinforcing phase [4–9]. Most of the investigations focused on relatively small (<30 vol.-%) filling degrees [10–13]. In 1963, Hill investigated the theoretical principles of elastic properties of reinforced solids [4]. Wang studied the modulus of porous materials [5]. In 1990, Ahmed and Jones reviewed the published theories and demonstrated the limitations of the existing theoretical models, which

* Corresponding author at: Institute of Solids Process Engineering and Particle Technology, Hamburg University of Technology, Hamburg, Germany. Tel.: +49 40 42878 2811; fax: +49 40 42878 2678.
E-mail address: michael.wolff@tuhh.de (M.F.H. Wolff).

0032-5910/$ – see front matter © 2013 The Authors. Published by Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.powtec.2013.07.009

do not yet consistently reproduce the experimental findings [6]. Very little dependence of the modulus of elasticity on the mean particle diameter was found by Spanoudakis and Young for particles of sizes from 10 to 60 μm and filling degrees between 10 and 46 vol.-% [14], and by Verbeek for particle sizes between 60 and 340 μm and a filling degree of 50 vol.-% [15]. LLorca et al. developed a roadmap for the multiscale simulation of composite materials, but focused on the simulation of fiber-reinforced composites [16].

In 2008, Fu et al. reviewed the effects of particle size and particle/matrix interface adhesion on the mechanical properties of particulate-reinforced composites with focus on small aspect ratios of the reinforcing phase [8]. They found that both strength and fracture toughness were influenced by all examined parameters, while the modulus of elasticity is significantly dependent only on the filling degree. In this paper, the micromechanical behavior of ceramic–polymer composite materials under bending is investigated using the discrete element method (DEM). With this method, it is possible to account for the discrete nature of the material on the microscale. Each ceramic particle is modeled as one discrete element, and the polymeric binder between the particles is modeled as solid bonds between these elements. Unlike most other modeling approaches, such as Finite Element Method (FEM), the particulate structure, particle size distributions and packing structure, and the pore structure are naturally considered and can be adjusted to match the desired structures.

2. Simulation method

2.1. Discrete element modeling

Since its emergence in the 1970s [17], the discrete element method (DEM) has developed into one of the primary techniques for modeling various kinds of particulate systems and processes. In the DEM, solid material is simulated as discrete and indestructive elements, which interact with each other via contact forces. The forces acting on each particle include contact forces between particles, solid bonds between particles, pressure gradients, drag, gravity, adhesive forces, etc. The forces and moments are summed up, and then they are used to numerically solve Newton's and Euler's equations of motion for individual simulation time steps. In recent years, DEM has been used to model a variety of ceramic processes and applications, including compaction of ceramic powders [18], compression tests [19,20], sintering of ceramics [21–23], modelling of fibre composites [24], and studies on two-dimensional cantilevers [25]. The DEM has been reviewed, among others, by Zhu et al. [26,27]. It has also been coupled with computational fluid dynamics to model fluidized bed processes [28–30]. However, hardly any study can be found in literature which deal with the bending or tensile testing of materials using DEM. Recently Nohut [31] studied the influence of grain size on fracture toughness of ceramics in 2D using DEM. Kempton et al. [32] investigated the compression and tensile deformation behavior of agglomerates using a sub-particle DEM õapproach, meaning that the tested agglomerates consisted of smaller particles held together by adhesive contact forces and solid bonds.

2.2. Generation of the modeled structure

The material which was modeled as the discrete particles was a ceramic material such as α-Al_2O_3, which has a density at room temperature of about 3.98 g/cm^3, a shear modulus of about 169 GPa, and a Poisson ratio of 0.23 [33]. These parameters were used as input parameters to calculate the contact force between overlapping particles. It was calculated according to the Hertz-Mindlin-Tsuji model [34–36], as summarized e. g. in [30]. Due to the linear-elastic nature of the modeled ceramic particles and the quasi-static conditions during the loading, the particle deformation is dominated by the elastic part. Thus, the coefficient of restitution was set to between 0.8 to 1 in all simulations, corresponding to a linear-elastic contact with little damping. In order to reach a high packing density without residual stresses after compaction, each particle with physical radius r_i was generated with an additional shell of thickness 6 μm, leading to a contact radius r_i^c of $r_i^c = r_i + 6$ μm. The thickness of the shell was empirically chosen, and other values can be used. However it should be clearly smaller than the particle radius, and large enough to avoid physical overlap. A contact between two particles i and j with position vectors $\vec{P_i}, \vec{P_j}$ and radii r_i, r_j was detected when the condition $\left(r_i^c + r_j^c - \left|\left(\vec{P_i} - \vec{P_j}\right)\right| \geq 0\right)$ was met (Fig. 1). For each contact the normal overlap

$$\delta_{n,ij} = r_i^c + r_j^c - \left|\left(\vec{P_i} - \vec{P_j}\right)\right| \quad (1)$$

was calculated using the contact radii r_i^c and r_j^c during the compression phase. After compression and before bond generation, the radii entering Eq. (1) were changed to the physical radii. The contact force at bond generation time $t = t_b$ was thus eliminated for almost all contacts, corresponding to a stress-free state of the specimen.

To include the contact force between contacting particles, the elastic part of the contact force was calculated according to the elastic part of the Hertz model as

$$F_n = \frac{4}{3} E^* \sqrt{r^*} \delta_n^{3/2} \quad (2)$$

using the equivalent modulus of elasticity E^* and equivalent radius r^* [30]. This force was added to the solid bond force. At $t = 0$s, the particles were generated with a size distribution shown in Fig. 2. The number of particles N was limited to 9,500 to reduce computational effort. The resulting specimens had a length on the mm-scale, which is about one order of magnitude smaller than typical sample sizes for mechanical bending tests (cm-scale). However, while the strength of brittle materials typically decreases with the sample size, no appreciable dependence of the modulus of elasticity on the sample size is to be expected for the composite structure within this size range. The particle size distribution was chosen in such a way that it models a μm-structured filler material with a mean particle diameter $d_{50,3}$ ~ 31 μm (Fig. 2). The solid volume of the sample was 0.151 mm^3. For the generation, the particles were randomly distributed in a large box ($V_{box}/V_{particles} = 132$) and then compressed by successively decreasing the box volume, until a cuboid of height $h = 256$ μm, width $w = 235$ μm and length $L = 4.27$ mm (volume $V_{specimen} = 0.257$ mm^3) was reached (Fig. 3).

The packing density ρ was determined in the following way: First a cuboid of certain size was defined within the specimen. The volume of all particles whose centres were located within this volume were summed up, and this was divided by the total volume of the chosen cuboid. This was done for several cuboid sizes and the resulting average packing density was about 63%. By doing so, the effect of the surface on the packing density could be eliminated and the true bulk density was determined.

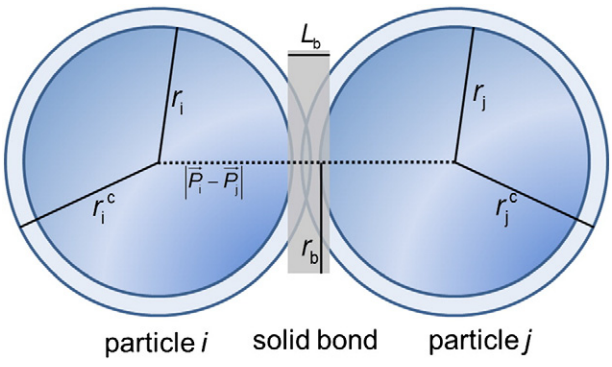

Fig. 1. Sketch of a contact with bond between two particles i and j.