European Journal of Mechanics A/Solids 59 (2016) 252–264

Contents lists available at ScienceDirect

European Journal of Mechanics A/Solids

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

Elastic properties of solid material with various arrangements of spherical voids

Sascha Heitkam [a, *], Wiebke Drenckhan [b], Thomas Titscher [c], Denis Weaire [d], Daniel Christopher Kreuter [e], David Hajnal [f], Frederic Piechon [b], Jochen Fröhlich [a]

[a] Institute of Fluid Mechanics, Technische Universität Dresden, 01069 Dresden, Germany
[b] Laboratoire de Physique des Solides, CNRS, Universit Paris-Sud, 91405 Orsay, France
[c] BAM Federal Institute for Materials Research and Testing, 12205 Berlin, Germany
[d] School of Physics, Trinity College Dublin 2, Ireland
[e] Institut für Festkörpermechanik, Technische Universität Dresden, 01307 Dresden, Germany
[f] BASF SE, 67056 Ludwigshafen, Germany

ARTICLE INFO

Article history:
Received 5 October 2015
Received in revised form
6 April 2016
Accepted 7 April 2016
Available online 10 April 2016

Keywords:
Void material
Young's modulus
Poisson ratio
Foam
Finite element method

ABSTRACT

In this work the linear elastic properties of materials containing spherical voids are calculated and compared using finite element simulations. The focus is on homogeneous solid materials with spherical, empty voids of equal size. The voids are arranged on crystalline lattices (SC, BCC, FCC and HCP structure) or randomly, and may overlap in order to produce connected voids. In that way, the entire range of void fraction between 0.00 and 0.95 is covered, including closed-cell and open-cell structures. For each arrangement of voids and for different void fractions the full stiffness tensor is computed. From this, the Young's modulus and Poisson ratios are derived for different orientations. Special care is taken of assessing and reducing the numerical uncertainty of the method. In that way, a reliable quantitative comparison of different void structures is carried out. Among other things, this work shows that the Young's modulus of FCC in the (1 1 1) plane differs from HCP in the (0 0 0 1) plane, even though these structures are very similar. For a given void fraction SC offers the highest and the lowest Young's modulus depending on the direction. For BCC at a critical void fraction a switch of the elastic behaviour is found, as regards the direction in which the Young's modulus is maximised. For certain crystalline void arrangements and certain directions Poisson ratios between 0 and 1 were found, including values that exceed the bounds for isotropic materials. For subsequent investigations the full stiffness tensor for a range of void arrangements and void fractions are provided in the supplemental material.

1. Introduction

Introducing spherical voids into a solid and otherwise homogeneous and isotropic material changes its mechanical properties significantly. Such materials are currently generated using templating techniques (Yin et al., 2012), by integrating hollow spheres in a matrix (Kenig et al., 1985) or by direct foaming (Testouri et al., 2010, 2012). The voids of the resulting material can be arranged in an ordered or in a disordered manner. It is therefore of considerable interest to compare the mechanical properties of different ordered and disordered void structures, including the case where the voids overlap.

When direct foaming is used, the equal-volume bubbles tend to organize themselves on a close-packed lattice in densest packing (Heitkam et al., 2012). Depending on the precise method of generation, the void arrangement may be chosen to be dominated by FCC (face-centred cubic) or HCP (hexagonal close-packed) arrangement (Heitkam et al., 2012; Drenckhan and Langevin, 2010). This raises the practically relevant question whether one of these arrangements should be preferred over the other, due to advantageous mechanical properties of the resulting solid void material.

Porous materials show a very rich range of non-linear mechanical behaviour, including plastic deformation, buckling and rupture. Here, we concentrate on the linear elastic behaviour, corresponding to infinitesimally small strain. The complementary

* Corresponding author.
E-mail address: sascha.heitkam@tu-dresden.de (S. Heitkam).

http://dx.doi.org/10.1016/j.euromechsol.2016.04.003
0997-7538/

problem, the elastic properties of crystalline arrangements of solid spheres, has been investigated experimentally and numerically by several authors (Radjai et al., 1999; O'Hern et al., 2001; Mueggenburg et al., 2002; Sanders and Gibson, 2003; Ngan, 2004; Yin et al., 2012; An and Yu, 2013). The elastic properties of the void material of these packings, however, have not yet been investigated sufficiently and comparatively.

Before computers made their breakthrough in science, the elastic properties of void material were estimated by superposition of the effects of a single void (Hill, 1965; Budiansky, 1965; Iwakuma and Nemat-Nasser, 1983). These methods yield good results for low void fraction. However, with increasing void fraction, higher orders of interaction between the voids have to be taken into account (Eischen and Torquato, 1993; Torquato, 1997, 1998). Christensen (Christensen, 1990) compared different micro-mechanic models available at that time. In 1992, Day et al (Day et al., 1992). developed a simple Finite Element Method (FEM) to calculate the elastic properties of a two-dimensional material with circular voids. They investigated the influence of void fraction and topology separately and devised a simple analytical explanation for the calculated values. After 1992, increasing computer power became available for many research groups, resulting in further direct numerical simulations of the interstitial material of sphere or bubble arrangements in three dimensions (Segurado and Llorca, 2002; Ni and Chiang, 2007; Bouhlel et al., 2010; Saadatfar et al., 2012). In 2006, Ni et al (Ni and Chiang, 2007). calculated the Young's modulus of a simple cubic void structure and compared their results to analytical estimations of (Iwakuma and Nemat-Nasser, 1983) and (Cohen, 2004), which are used later for comparison.

The agreement between analytical (Cohen, 2004; Iwakuma and Nemat-Nasser, 1983) and numerical (Ni and Chiang, 2007) methods was very good. However, the graphs of Young's modulus versus void fraction depend only weakly on the structure. Thus, small derivations between the graphs raise the question, as to whether a difference results from the uncertainty of the method or rather from the structural differences of the investigated materials. In order to reliably extract the structural effects, one therefore needs to apply an identical numerical method to different structures, taking great care of the numerical uncertainty. Additionally, many of the available studies are confined to low or medium void fractions.

In this paper, a comparative study of a wide variety of dense sphere packings is carried out, revealing the influence of the structure on the elastic properties. The entire range of void fractions is considered, as illustrated in Fig. 1. Small voids form closed-cell void material with low void fraction. Retaining the regularly arranged void centres and increasing the diameter the voids touch each other at a certain void fraction $\phi_{tv,ouch}$, forming closed-packed void material. At even higher void fractions, the voids overlap, forming open-cell void materials.

2. Material and methods

2.1. Definition of sphere structures

Monodisperse spheres or microbubbles tend to crystallise when they become agglomerated. This means that their centres form a periodic, crystalline lattice. Since these systems strive for densest packing, they are usually arranged in the hexagonally close-packed (HCP) or face-centred cubic (FCC) structure, both providing equally dense sphere packings (Weaire and Aste, 2008). For comparison, simple cubic (SC) and body centred cubic (BCC) arrangements are also taken into account here. If the spheres are slightly polydisperse or if the agglomeration process is too fast to allow for relaxation, random closed-packed (RCP) structures are created.

From the different structures mentioned above, rectangular or cubic representative volume elements (RVE) were derived which are shown in Fig. 2. Except for SC, the RVE does not coincide with the primitive cell of the crystalline arrangements. Rather, it is the smallest cuboid cell which may be periodically combined to represent the complete structure, because the numerical method only allows for orthogonal, periodic boundaries. Parameters of the chosen RVE are given in Table 1. Note that for FCC two different RVEs were applied and compared. The cubic RVE, labelled FCC, is a cube, bounded by planes in (100), (010) and (001). The hexagonal RVE, labelled FCCh, is a cuboid, bounded by (111), $(1\bar{1}0)$ and $(11\bar{2})$ planes. This provides an additional test of the method applied by comparing the Young's moduli of the different RVE of the same structure. This is explained in more detail in Section 2.4 below. The RCP structure is special, since it does not correspond to a crystalline lattice, but it does involve periodic boundary conditions. The sphere positions for this case were generated using a gas-dynamic algorithm that is freely available (Skoge et al., 2006). Drugan et al (Drugan and Willis, 1996; Drugan, 2000). found, that with six spheres in an RVE of disordered voids, the statistical uncertainty of the mechanical properties is below 5%. Aiming for very high accuracy, here RVEs with 30 spheres were generated. The statistical uncertainty resulting from this type of RVE was investigated, as reported in Section 2.4 below.

The solid fraction $\phi_s = V_{solid}/V_{RVE}$ of a void material is the ratio of the volume of solid material V_{solid} contained in a given RVE with the volume V_{RVE}. The void fraction $\phi_v = 1 - \phi_s$ is the ratio between the void volume V_{void} and the total volume of the RVE. In case of separated spherical voids, the void volume can be calculated from the sum of the volume of each spherical void contained in a given RVE. In this case, the void fraction depends on the sphere diameter D, the lattice spacing L, and the packing density $\phi_{v,\text{touch}}$ for touching spheres of the structure considered

$$1 - \phi_s = \phi_v = \frac{V_{void}}{V_{RVE}} = \phi_{v,\text{touch}} \left(\frac{D}{L}\right)^3 = \phi_{v,\text{touch}} \left(1 - \frac{l_l}{L}\right)^3. \quad (1)$$

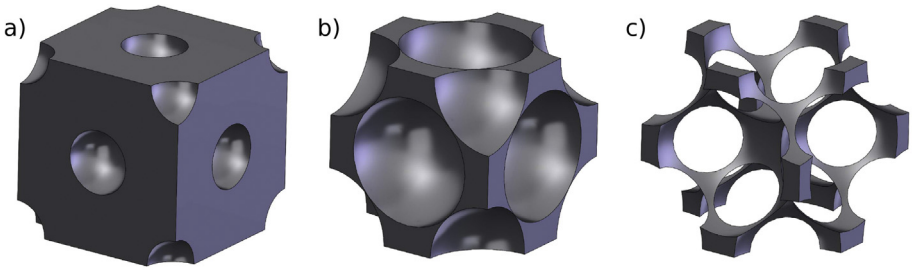

Fig. 1. Void material with spherical voids of equal size in face-centred cubic arrangement at different void fractions. a) closed-cell structure at $\phi_v = 0.09$, b) touching spheres at $\phi_v = 0.74$ and c) open-cell structure at $\phi_v = 0.95$.