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Original Article

3D microstructure-based modelling of the deformation behaviour of ceramic matrix composites

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ABSTRACT

In this paper the experimental and numerical investigations of microstructure modelling of multilayer actuator are considered. $BaTiO_3$ powder is manufactured using the solid-state technique. The main parameter influencing the possibility of application of $BaTiO_3$ ceramics on actuators is the grain size of the sintered materials. Three kinds of pellets with different average grain sizes were considered. The adhesive joints of a $BaTiO_3$ and Ag-based conducting electric current epoxy adhesive were used to fabricate the model of actuator. A 3D microstructure model of $BaTiO_3$ and composites were generated using Digimat-FE software. The Mori–Tanaka and double inclusion homogenization models for representative volume elements of multilayer actuator were carried out using Digimat-MF software, in order to obtain the failure characteristics of the composite material. To investigate the failure of the ceramic matrix composite the Hashin-Rotem criterion was used.

1. Introduction

Barium titanate ($BaTiO_3$) is a fundamental ferroelectric perovskite structure and is a widely used piezoelectric ceramic material. The mechanical and physical properties of $BaTiO_3$ are wide-ranging and depend on its grain size [1,2]. Several studies [i.e., 1, 3] have been carried out to investigate the effect of micro- and nano-size fine powders, the compaction method, and sintering conditions on the properties of $BaTiO_3$. The ceramics microstructure influences the dielectric properties of electro-mechanically coupled materials [4]. The piezoelectric effect causes this by applying a mechanical load to these materials so that an electric field is produced. Under an inverse piezoelectric effect the piezoelectric ceramics exhibit a mechanical deformation in response to an external electric loading [5]. Owing to these smart properties of piezoelectric materials, $BaTiO_3$ is often used in sensors, transducers and multilayer ceramic capacitors, because of its high dielectric constant and low loss characteristics. Piezoelectric ceramics are used widely in a variety of applications in automotive engineering, civil and mechanical engineering, actuators and medical technology and consumer applications.

To analyse the fracture and residual stresses in ceramal, analytical, empirical and numerical methods were used. For the stress state analysis in composite materials, including ceramics, a number of methods were used, including a shear lag model and the Eshelby model [6]. The use of analytical methods may lead to results that differ significantly from the results of experimental research, whereas experimental investigations are costly. Therefore, it is helpful to use numerical methods. Finite Element Analysis (FEA) is currently the most commonly used numerical method for the physical discretization of materials. The Finite Element Method (FEM) requires discretization of the entire area of the analysed body, which adversely affects the analysis time. To reduce the computational time, two-dimensional models of the orthotropic microstructure of ceramics are often used in the finite element analysis. Tvergaard and Hutchinson [7] proposed a two-dimensional model of the area, which is a triangular sector of three neighbouring hexagonal grains. Taking into account the spatial complexity of interactions between the orthotropic grains in a polycrystalline microstructure, three-dimensional models were developed [8].

It may be more advantageous to use the Boundary Element Method (BEM), which only requires the discretization of the edge of the analysed system and the use of the Green functions in the continuum domain. The boundary element method is a widely used approach to study nucleation and propagation crack in piezoelectric ceramics [9,10]. Denda [11] used a BEM for the analysis of semi-permeable piezoelectric cracks, based on the numerical Green's function approach.

Homogenization is an efficient method to predict the macroscopic behaviour of composite materials or aggregates. Homogenization allows the determination of the stress state in the ceramic material, on both the macro- and microscale. Analytical methods of homogenization for the composite materials, such as the Uniform Field Method (UFM)

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[12] and the Asymptotic Homogenization Method (AHM) [13], can be applied to obtain the effective properties of the ceramic-based transducer, based on the properties of its components. AHM can provide equivalent homogeneous volume, which describes the global behaviour of the material structure. However, finite element modelling is more efficient than modelling a complicated heterogeneous structure [14]. UFM is a generalization of the rules of mixtures which use parallel and series additions to model effective properties of two-phase materials [12]. The fundamental assumption of this method is that different selected fields are uniform with regard to the constituents of the heterogeneous media.

Among the homogenization techniques, the FE^2-based homogenization approach [15,16] is computationally efficient and capable of determining consistent homogenized physical quantities (stress, strain) and homogenized material quantities (stiffness tensor) [5]. However, the application of micro-boundaries in a small strain setting for homogenization does not generate a physically consistent Eshelby stress tensor. In an FE^2-based homogenization technique used for the homogenization of piezoelectric materials, a Representative Volume Element (RVE), comprises of the micro-structural features of the material, is assigned to every Gauss point of the macro-domain (Fig. 1). An application of this FE^2-based method towards the piezoelectric materials can be found in Schröder and Keip [17].

In previous decades some software and numerical algorithms for the realistic prediction of the non-linear constitutive behaviour of multiphase materials have been developed (Abaqus, MSC.Marc, Digimat). Digimat, used in this study, works via two main approaches to homogenization: the FEA-based homogenization approach (Digimat-FE); and the mean-field approach (Digimat-MF), such as the Mori–Tanaka and double-inclusion approaches. The direct finite element analysis in Digimat-FE (e-Xstream Engineering, Käerjeng, Luksemburg) on RFEs can generate accurate and detailed field results. So, it is a useful technique for modelling complex material microstructures [18–20]. Digimat-MF is the Mean-Field Homogenization (MFH) tool to rapidly compute the macroscopic performance of composite structures from their microstructure definition and per-phase properties [18]. The double-inclusion model (Fig. 2a), as proposed by Nemat-Nasser and Hori [21] and Hori and Nemat-Nasser [22], consists of an ellipsoidal inclusion embedded in another ellipsoidal matrix. The tensor of strain concentration for the inclusion (Ω) and the matrix phase (Γ) of the double-cell are taken for each inclusion. The orientation and shape of the inclusion and the matrix, and the elastic properties of these three phases are arbitrary [23]. Such an approach provides great flexibility and can be used to evaluate the effective properties of a two-phase composite with different inclusion arrangements. For non-dilute inclusions, the Mori–Tanaka scheme [24] allows the efficient evaluation of the properties of multiphase materials, covering a wide variety of inclusion shapes and distributions. The ellipsoidal inclusions are randomly orientated in the domain space. The shape and orientation of each double-cell are identical to those of the inclusion enclosed in it (Fig. 2b).

Mean-Field Homogenization methods (i.e., Mori–Tanaka method [24], Lielens method [25]) were the first to be developed in the framework of linear elasticity [26], and are able to predict, among other properties, the elastic constants [26]. Using these methods, a local problem for a single inclusion is solved in order to obtain approximations for the local field behaviour, according to Eshelby's inclusion [27]. Next, the local fields are averaged to obtain the global ones.

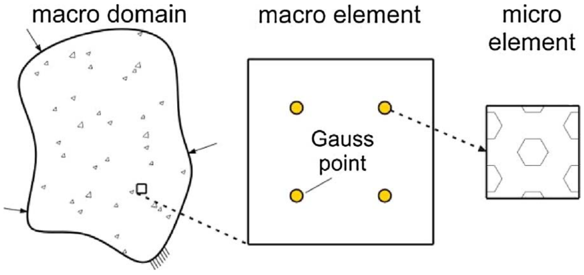

Fig. 1. Macro-micro transition.

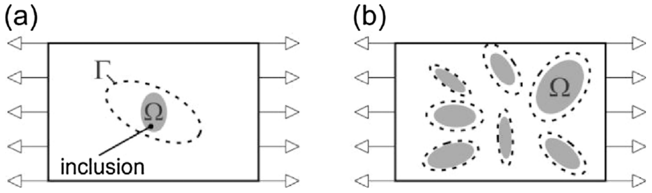

Fig. 2. Schemes of (a) double-inclusion and (b) Mori–Tanaka methods.

Existing methods for modelling ceramic structures can be used for the complex studies of ceramic matrix composites, polymer matrix composites, piezoelectric macro-fibre composites, and others ceramal materials [28–31]. A detailed survey of homogenization approaches can be found in the articles by Kanouté et al. [32] and Geers et al. [33]. A comprehensive overview of homogenization methods is provided by Nemat-Nasser and Hori [21].

In this paper, three kinds of BaTiO$_3$ pellets and cylindrical specimens were fabricated from powder milled at different time and sintered at various maximal temperatures. The modelling of layers of the multilayer actuator (MLA) consisted of barium titanate ceramic layers, bonded by using Ag-based conducting electric current epoxy adhesive, was carried out using Digimat-FE software. Two homogenization models (Mori–Tanaka and double inclusion) were applied to model the fracture of the representative volume element of the actuator model. The Hashin-Rotem criterion was used for the failure prediction of the ceramic matrix composite.

2. Experimental

2.1. Barium titanate powder and granulate

The powder of barium titanate (BT) perovskite was fabricated from TiO$_2$ (99% purity, Kronos) and BaCO$_3$ (99.5% purity, Chempur) using the solid-state method. The mechanical activation of raw materials together with isopropyl alcohol took place in a mixer mill with a working chamber of Ø135 × 180 mm for 2 h, with a rotation of 280 min^{-1}. As a grinding medium, zirconia balls of 4.5 kg in weight were employed. The obtained slurry was dried at 70 °C and the calcination of the powder was carried out in an electric furnace at the maximal temperature of 1100 °C. The temperature increased at a speed of 100 °C/h, the dwell time was equal to 8 h, and the speed of cooling was 100 °C/h until 800 °C, after which free cooling took place at room temperature. Triple mechanical activation and calcination were necessary to obtain the monophase BaTiO$_3$ material. This powder was treated as the basis, and denoted as powder 'a'.

BaTiO$_3$ powder 'a' was granulated in order to improve mouldability. Powder 'a' was milled with deionized water in a 1:1 ratio in a porcelain mill for 30 min. Then the following components were added: 0.2% dispex (BASF), 0.2% oil emulsion F15 (Naftochem) and 1% polyvinyl alcohol PVA (Japan Vam & Poval). The granulation process was performed in a spray drier (Niro), together with a peristaltic pomp type 372C, with an inlet temperature of 220 °C, an outlet temperature of 80 °C and spray pressure equal to 40 mm water column. The obtained granulate was denoted as granulate 'a'.

2.2. Pellets and cylindrical specimens fabrication

Pellets and cylindrical specimens for the compression test were obtained in a mould with an external diameter of 11.5 mm, where BaTiO$_3$ granulate 'a', with a weight of 0.3 g and 12 g for pellets and