ANALYSIS OF CRACK INITIATION AND PROPAGATION IN A PIEZOELECTRIC CERAMIC USING THE BOUNDARY ELEMENT METHOD

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Abstract
The subject of this paper is the analysis of crack initiation and propagation in barium titanate ceramic using the boundary element method. In micro-mechanical analyses, it is very important to have information on the real microstructure of a material. A barium titanate pellet was prepared using a solid-state technique. The boundary element method is used so that it can be combined with three different grain boundary formulations for the investigation of micro-mechanics as well as crack initiation and propagation in a piezoelectric actuator. In order to develop a numerical programming algorithm, suitable models of polycrystalline aggregate and representative volume elements have been prepared for boundary element analysis.

Keywords: barium titanate, boundary element method, ceramics, microstructure

1 Introduction

A The boundary element method (BEM) is one of the favourite optimised numerical computational methods used by scientists in many areas of engineering and science including fracture mechanics, fluid mechanics, and geology. In order to use the boundary element method, one only needs to fit the boundary of the system without calculation of parameters inside the solid body analysed, so the dimension of the problem can decrease and the size of the algebraic equations can be considerably smaller than the finite element equation [1, 2].

In the area of fracture mechanics and mechanical engineering, some researchers have utilised the boundary element method [3, 4], the Voronoi tesselation method [5] or the finite element method [6, 7]. These methods are very suitable for use in determining the behaviour of a solid body which contains several cracks and holes. It is worth mentioning that both finite and infinite bodies can be studied via the BEM. In order to use this method, one must pay attention to the fact that the traction fundamental solution and displacement fundamental solution for isotropic bodies are different to those for anisotropic bodies. This is the most important fact that researchers have to consider before using the BEM [8, 9] or discrete element method [10] for investigations. The application of the boundary element method in micromechanics and multiscale modelling has been studied by a number of researchers [11-13]. In some of these studies, researchers only modelled materials at micro scale and with the cohesive law, averaging theory or nonlocal theories were not used. Several researchers have utilised some basic concepts

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of micro mechanical analysis such as representative volume element and grain boundaries in their studies [14].
In this paper the analysis of crack initiation and propagation in barium titanate ceramic is analysed using the boundary element method. The boundaries of grains were compared to the real microstructure of barium titanate ceramic.

2 Experiment

The barium titanate pellet was prepared using the solid-state method [15, 16]. The barium titanate powder was manufactured from 288.15 g of TiO_2 (99% purity, Kronos) and 711.85 g of $BaCO_3$ (99.5% purity, Chempur). The three calcinations of $BaTiO_3$ powder were carried out in an electric furnace. In order to improve mouldability, the barium titanate powder thus obtained was granulated. $BaTiO_3$ powder with a weight of 3962 g was milled with deionised water in the proportion 1:1 in a porcelain mill with a 3 kg ball for 30 minutes. The granulation process was performed in a spray drier (Niro). The pellets were pre-formed by filling the mould for uniaxial pressing with an external diameter of 11.5 mm with $BaTiO_3$ granulate with a weight of 0.6 g followed by uniaxial pressing under a pressure of 1 MPa. The microstructure of the $BaTiO_3$ powder has been evaluated using a scanning electron microscope SEM/HITACHI S-3400N/2007.

3 Theoretical background

In this paper both the macro and micro scales are analysed. Modelling, often on a macro-scale, is based on micro-continuum theories; however, it is necessary to pay attention to the point that in order to preserve the integrity of the material, no constitutive law or damage should be considered. In the next step, by applying the boundary condition on a representative volume element (RVE) which was obtained from calculations at macro scale, the cohesive laws can be reevaluated for the modelling of crack initiation and propagation in the RVE. The RVE is a small volume of microstructure that has the general characteristics of the whole microstructure such as the volume fraction, morphology and randomness of the phases and over which modelling of specific characteristics is carried out [17]. All information from the micro-scale can be sent to the macro level to modify the results and model the next steps. In **Fig. 1** it is shown that the calculation of the micro-scale is able to provide boundary conditions for the micro-scale, on the other hand, the micro scale will provide some information by which the constitutive law can be modified and possible damage can also be modelled for the next steps.

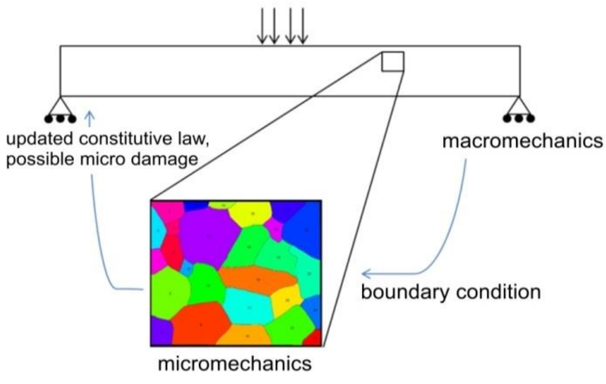

Fig. 1 Schematic view of multi-scale tension modelling

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4 Application of BEM at macro scale

In order to perform the procedure for multiscale modelling, the existence of micro-cracks which can appear due to a pre-existing manufacturing process or can be created during external loads, results in a decrease in the materials' stiffness in macro and meso scale. If we consider the boundary element method as a means for solving this problem, nonlinear behaviour may occur [18]. Thus, it is necessary for the macro scale to be simulated via a nonlinear boundary element formulation in order to exploit the local nonlinear behaviour of the material. The boundary element formulation is as follows [19]:

$$\frac{1}{2}u_i(Z_0) = \int_s U_{ij}(x,Z_0)\,t_j(x)\,ds(x) - \int_s T_{ij}(x,Z_0)\,u_j(x)\,ds(x) + \int_V E_{ijk}(X,Z_0)\sigma_{jk}^D(X)\;dV \tag{1.}$$

σ_{jk}^D is decremental stress which is posed by the micromechanical solution in order to treat the local softening of stress in macroscale. E_{ijk} is a fundamental solution for the initial stress which can be defined as a stress at point X for unit point load which is applied at point Z_0. In the literature, there are many references which provide the E_{jk} (X, Z_0) for isotropic materials, however, in this paper, piezoelectric materials are considered as anisotropic both in macroscale and at microscopic scale and according to experience, there is no information in the literature to apply this formulation to anisotropic materials. So, in order to achieve accurate results, it is essential to define the fundamental solution for the stress for anisotropic materials. These equations define the stress and displacement using Stroh formulations:

$$u = 2\,\mathrm{Re}\left\{\sum_{k=1}^{4} a_k\, f_k(z_k)\right\},\ \phi = 2\,\mathrm{Re}\left\{\sum_{k=1}^{4} b_k\, f_k(z_k)\right\} \qquad \sigma_{i1} = -\phi_{i,2},\quad \sigma_{i2} = \phi_{i,1} \tag{2.}$$

By differentiation of u with respect to z_k, the strain can be defined as:

$$\varepsilon_{ij} = 2\,\mathrm{Re}\left\{\sum_{k=1}^{4} a_k(\delta_{1j} + p_\alpha \delta_{2j})\, f_k'(z_k)\right\} \tag{3.}$$

In order to define the fundamental solution for strain, we need to consider an infinite anisotropic plate under a concentrated force applied at $Z_0(x_{01}, x_{02})$ as shown in **Fig. 2**. By considering the following boundary condition, the elastic solution of this problem will be considered as the Green function for the fundamental solution of the boundary element method.

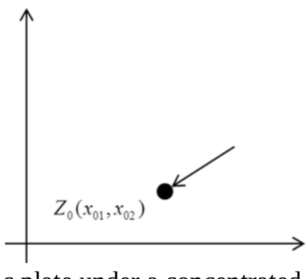

Fig. 2 An infinite anisotropic plate under a concentrated force applied at $Z_0(x_{01}, x_{02})$

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The boundary condition can be written as:

$$\begin{aligned}&\int_C d\phi = f \quad \text{any closed curve enclosing point } Z_0\\&\sigma_{\mathrm{ij}} \to 0 \text{ at infinity}\end{aligned} \tag{4.}$$

Now to solve Eq. (2.), it is critical to allocate a function to *f*. In the literature, the following function is proposed for *f*:

$$f_k(z_k) = \log(x_k - Z_{0k}), \tag{5.}$$

So, the displacement and stress function can be written as:

$$u = 2\,\mathrm{Re}\left\{\sum_{k=1}^{4} \mathbf{AF}_k(\mathbf{z}_k)\mathbf{q}_k\right\},\ \phi = 2\,\mathrm{Re}\left\{\sum_{k=1}^{4} \mathbf{BF}_k(\mathbf{z}_k)\mathbf{q}_k\right\} \tag{6.}$$

where

$$\begin{aligned}&\mathbf{A} = [\mathbf{a_1} \quad \mathbf{a_2} \quad \mathbf{a_3} \quad \mathbf{a_4}],\ \mathbf{B} = [\mathbf{b_1} \quad \mathbf{b_2} \quad \mathbf{b_3} \quad \mathbf{b_4}]\\&\mathbf{F}_k(\mathbf{z}_k) = diag[f_k(z_k)] \quad k = 1,2,3,4\end{aligned} \tag{7.}$$

Now, by applying the boundary condition to a model, Eq. (7.) can be represented as:

$$\begin{aligned}&2\,\mathrm{Re}\{i\mathbf{Bq}_0\} = f/2\pi,\\&2\,\mathrm{Re}\{i\mathbf{Aq}_0\} = 0.\end{aligned} \tag{8.}$$

By using the orthogonality relation among eigenvectors

$$\begin{bmatrix}\mathbf{A}^{\mathrm{T}} & \mathbf{B}^{\mathrm{T}}\\ \overline{\mathbf{A}}^{\mathrm{T}} & \overline{\mathbf{B}}^{\mathrm{T}}\end{bmatrix}\begin{bmatrix}\mathbf{B} & \overline{\mathbf{B}}\\ \mathbf{A} & \overline{\mathbf{A}}\end{bmatrix} = \mathbf{I} \tag{9.}$$

5 Results and discussion

As is obvious in **Fig. 3**, the numerical algorithms used act in a very efficient manner. Not only are the distances between the grains eliminated, but also in the corners, the grains have the same coordinates and this will increase the accuracy of the numerical models. **Fig. 4** shows crack initiation and propagation in the artificial grain used by Verhoosel and Gutiérrez [20]. In this example, uniform traction was chosen as the boundary condition. It can be concluded from this figure that the path of crack initiation which is predicted in the current work via the boundary element method and the introduction of cohesive law is almost the same as the one developed by Verhoosel and Gutiérrez [20].

Some small differences can be seen which are due to the different cohesive law along with the transgranular fracture that was predicted in [20]. Several assumptions are made to model the grain boundary in micro-scale. In the first step, before the cracks occur, the traction equilibrium and displacement compatibility are the governing equations. When the micro-crack starts to be initiated, the mixed mode potential based cohesive law is applied to the model grain boundaries and the intergranular crack nucleation and evolution is investigated.

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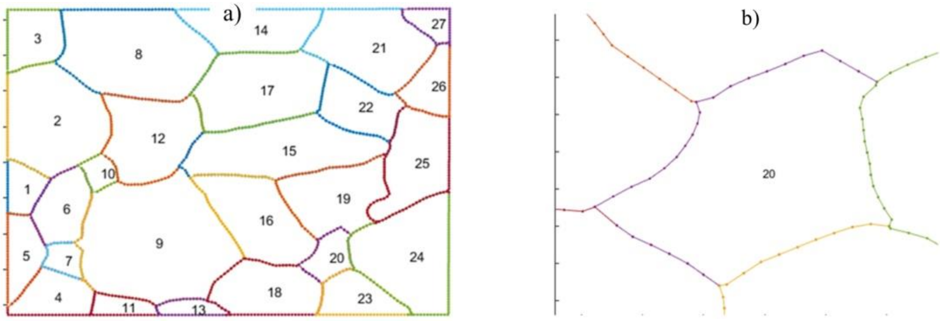

Fig. 3 Discretised grain boundaries in two different views, (a) larger view, (b) zoomed view of grain number 20 [20]

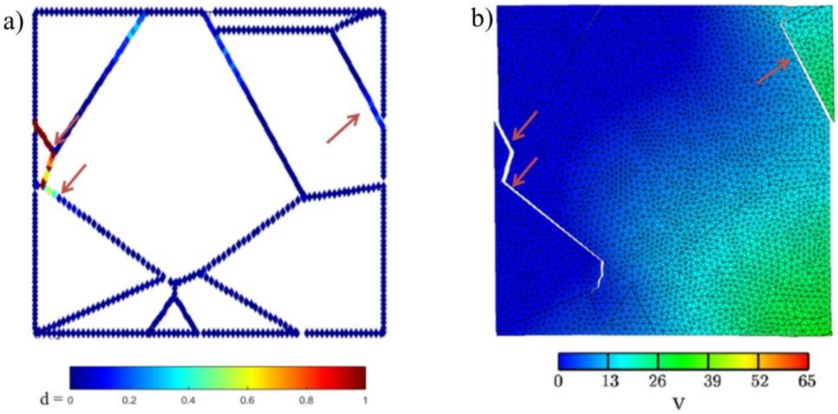

Fig. 4 The comparison between (a) the grain boundary algorithm developed and (b) Verhoosel and Gutiérrez [20] in predicting crack initiation and propagation

Upon interface failure, a frictional law is utilised in order to study separation, sliding or sticking between the micro-crack surfaces. Moreover, the model that was developed was validated by comparing the results with the literature. The influence of different parameters such as the piezoelectric effect, grain size and morphology, model domain, pre-excited cracks, metallic interface and frictional coefficient have been studied. The results indicate the efficiency of the proposed micro-mechanical model in the study of the advantages and disadvantages of the multilayer actuator.

Summary and conclusions

The structural model of RVE was obtained based on the microstructure of the $BaTiO_3$ ceramic that was prepared. The grain boundaries were divided into three zones, namely the undamaged zone, the cohesive zone and the failure zone and a suitable formulation for each zone was developed in order to study the behaviour of the RVE. The adaptive method developed for the investigation of the intergranular micro-fracture and micro-mechanical analysis of a homogenous and multilayer actuator was found to be a suitable algorithm by comparing some of the results with literature. The results of numerical analyses indicated that the type of load applied and the boundary conditions influence the fracture path of micro-structures which indicates that in different practical applications the type of external load must be considered to be an important factor. It can also be concluded that the piezoelectric coupling has a significant influence on the fracture criteria of aggregates which means that when considering the piezoelectricity and for a specified amount of strain, the polycrystalline aggregate without piezoelectric effect may experience more stress.

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