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Modelling of Barium Titanate Microstructure Based on Both the Boundary Element Method and a Homogenization Technique

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Abstract

This paper presents the results of research undertaken to develop a grain boundary element (BE) formulation for the micromechanical analysis of multilayer barium titanate ceramics. The BE formulation of the elastic problem is generated for single grains and polycrystalline aggregate of barium titanate ($BaTiO_3$) ceramics. In order to obtain $BaTiO_3$ powder, the solid-state technique was applied. The microstructure of sintered $BaTiO_3$ powder was examined in detail by scanning electron microscopy. Furthermore, image processing techniques and some numerical algorithms were employed to discretize the grain boundaries of ceramics. The single crystals of homogenous $BaTiO_3$ are represented as anisotropic elastic regions. A comprehensive numerical code is generated and image processing techniques are applied in order to discretize the boundaries of grains and obtain the exact coordinates of elements on the boundaries. Average thorium is developed to obtain the macro-stress and macro-strain. The numerical results show that the developed method is valid for analysing polycrystalline materials. The numerical investigations also show that the developed algorithm is accurate enough to investigate the mechanical properties of a multilayer piezoelectric actuator. It is also found that the position of the interface as well as the type of material plays an important role in determining the effective properties of the multilayer actuator.

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Keywords: Type your keywords here, separated by semicolons ; Barium titanate, Boundary element method, Homogenisation

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1. Introduction

In the area of fracture mechanics and mechanical engineering, the boundary element method (BEM) has been widely utilized. The BEM is one the favourite optimized numerical computational methods used by scientists in many areas of engineering and science including fracture mechanics, fluid mechanics, and electromagnetics. According to Groh and Kuna (2005), compared to the finite element method, the BEM demonstrates higher numerical stability and requires less computational resources. This BEM is very applicable in determining the behaviour of a solid body that contains several cracks and holes. It is worth noting 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 from those for anisotropic bodies. Cruse (1973) and Snyder and Cruse (1975) mention that this is the most important fact that researchers should consider when using the BEM for investigations and studies.

Pasternak (2012) and Yin (2000) noted that two main methods have been widely used by researchers to obtain the traction fundamental solution and displacement fundamental solution for anisotropic bodies. The first method is the use of Stroh's formulation, which is utilized in the current study, and the second one refers to Lekhnitskii's formalism. The most remarkable point that can be mentioned here with regard to the use of Stroh's formulation is the normalization of matrices, which will be mentioned in future chapters.

In order to use the BEM for analysing fracture problems, either a singular or a hypersingular integral has to be considered. Jafari et al. (2013) used only a singular integral, and via the derivatives of the basic equation of the BEM, they were able to analyse the dislocation density, which can be used for obtaining the stress intensity factor. On the other hand, through analytical transformations, integrals with strongly singular and hypersingular kernels were converted into weakly singular and regular integrals prior to any numerical evaluation. Garcia-Sanchez et al. (2005) used both linear element and quadratic elements for discretizing BEM over a body.

In order to obtain exact information about the behaviour of materials, it is necessary to estimate crack initiation and propagation on the micro-scale, which provides more accurate data for estimation of sensitive parts of materials along with the prediction of important curves such as the stress-strain curve or electrical potential-strain curve. Jafari et al. (2013) utilized micro-mechanical theories in finite element software, while others, such as Benedetti and Alibaldi (2013a, 2013b, 2015), generated numerical algorithms via the BEM to obtain the properties of materials.

In this paper, the boundary element formulation of an elastic problem is generated for single grains and polycrystalline aggregate of $BaTiO_3$ ceramics. A comprehensive numerical code is generated and image processing techniques are developed in order to discretize the boundaries of barium titanate grains and obtain the exact coordinates of elements along with the mechanical variables on the boundaries. Average thorium is developed to obtain the macro-stress and macro-strain. The numerical results show that the developed method is valid for analysing polycrystalline materials.

2. Experimental procedure

2.1. Synthesis of $BaTiO_3$

In order to obtain $BaTiO_3$ powder, the solid-state technique was applied. BT perovskite 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 set of raw materials was preliminarily mixed in a polyethylene beaker and then 1000 ml of isopropyl alcohol was added. The slurry obtained was dried in a drier at 70 °C, and calcination of the obtained powder was carried out in an electric furnace at a maximum temperature of 1100 °C for 8 hours, according to the calcination plan shown in Table 1. The received powder was then milled again for two hours together with 800 ml of isopropanol. This was followed by calcination of the obtained powder in an electric furnace at 1100 °C for 8 hours, according to the presented sintering curve. This second calcination cycle produced barium titanate powder that was milled for a third time for two hours. The third calcination of the obtained powder to produce $BaTiO_3$ was undertaken under the same conditions as employed in the previous two cycles.