

Micro-mechanical modelling of mechanical and electrical properties in homogeneous piezoelectric ceramic by using boundary integral formulations

M Biglar¹, F Stachowicz¹, T Trzpiecinski¹, M Gromada²

¹Rzeszow University of Technology, Faculty of Mechanical Engineering and Aeronautics, 35-959 Rzeszów, Poland

²Institute of Power Engineering, Ceramic Department CEREL, Research Institute, 36-040 Boguchwała, Poland

E-mail: m_biglar@prz.edu.pl

Abstract. Recent experiments on polycrystalline materials show that microcrystalline materials have a strong dependency on a grain size. In this study, mechanical and electrical properties of polycrystalline materials in micro level were studied by using averaging theorems. To completely understand the size-dependency of polycrystalline materials, an integral non-local approach that can predict the stress-strain relations for these materials was presented. In microcrystalline materials, crystalline and grain-boundary were considered as two separate phases. Mechanical properties of the crystalline phase were modelled using crystalline brittle material and is composed of randomly distributed and orientated single crystal anisotropic elastic grains. For microcrystalline materials, the surface-to-volume ratio of the grain boundaries is low enough to ignore its contribution to the elastic deformation. Therefore, the grain boundary phase was not considered in microcrystalline materials and mechanical properties of the crystalline phase were modelled using appropriate integral non-local approach. Finally, the constitutive equations for polycrystalline materials were implemented into a boundary integral equation and the results and some examples are provided for piezoelectric ceramic.

1. Introduction

During recent decades, application of piezoelectric ceramics such as actuator, sensors and transducers have been increased due to their efficiency in converting mechanical loads to electrical ones and viceversa. However, the most important problem is that piezoelectric ceramics are too fragile due to their special microstructural structures. That is why, during recent years, lots of researches were done in order to investigate microstructural properties of piezoelectric ceramics [1, 2].

There are different methods to understand the properties and behavior of materials. One of the most favorite methods that is receiving attentions of researcher during last years is multi-scale modeling which is able to model the properties of materials simultaneously at different alternative scales. Modeling a specific material at different scales at the same time makes it possible to study the behavior of heterogenous materials actually [3-5]. Due to the complexity of the material structure, there are no exact information about special characteristic of materials in a certain scale, therefore, one is able to determine these properties through a smaller scale. Thus, different classes of heterogeneous materials at different scales can be studied according to the same rules and the results can be compared



in order to achieve exact and actual behavior of materials [6]. Another advantage of multi-scale that can be mentioned is that damage evaluation can be predicted via this method overall different scale [7-9]. Damage models in multi-scale modeling are based on different theories. There are a lot of phenomenological and micromechanical models based on combination of quantities calculated at the macro-scale to evaluate damage.

2. Experimental

The macro-scale modeling is based on micro-continuum theories, however, paying attention to this point is necessary in order to save material integrity, no constitutive law or damage have to be considered. In the next step, by applying the boundary condition on a representative volume element (RVE) which was obtained from the calculation of macro scale, the cohesive laws can be brought up for modeling 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 volume fraction, morphology and randomness of the phases and over which modeling of specific characteristics is carried out [10]. All information from the micro-scale can be sent to macro level to modify the results and model the next steps. In Fig. 1 it is shown that the calculation of micro-scale is able to provide boundary conditions for micro-scale, on the other hand, micro scale will provide some information by which the constitutive law can be modified and possible damage can be modeled for next steps as well.

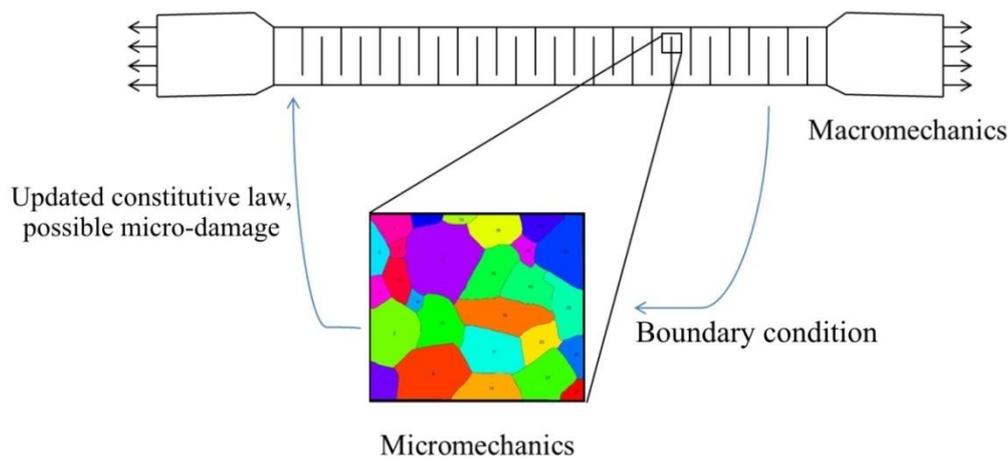


Figure 1. Schematic view of a multi-scale tension modeling

Via fundamental boundary element equation the displacement equation for each grain can be written as

$$\begin{aligned}
 & C_{ij}^H(z'_k) \tilde{u}_j^H(z'_k) + \int_{S_{nc}^H} \tilde{T}_{ij}^H(z'_k, z_k) \tilde{u}_j^H(z_k) dS_{nc}^H + \int_{S_c^H} \tilde{T}_{ij}^H(z'_k, z_k) \tilde{u}_j^H(z_k) dS_c^H \\
 & = \int_{S_{nc}^H} \tilde{U}_{ij}^H(z'_k, z_k) \tilde{t}_j^H(z_k) dS_{nc}^H + \int_{S_c^H} \tilde{U}_{ij}^H(z'_k, z_k) \tilde{t}_j^H(z_k) dS_c^H
 \end{aligned} \tag{1}$$

In equation (1), $\tilde{T}_{ij}^H(z'_k, z_k)$ and $\tilde{U}_{ij}^H(z'_k, z_k)$ are fundamental solution for traction and displacement which can be obtained via Stroh formulation for each grain. S_c^H and S_{nc}^H belong to boundary of internal grain and (contact boundary) and free boundary.

The overall volume average stress can be written according to averaging theorem as [11]:

$$\bar{\sigma}_{ij}^{m,t} = \frac{1}{V^m} \int_{S^m} x_i^m t_i^m dS^m \quad (2)$$

Where x_i^m and t_i^m are the position vector of points which are located on RVE boundary and their traction respectively. And the similar way, the volume average strain can be written as [11]:

$$\bar{\epsilon}_{ij}^m = \frac{1}{2V^m} \int_{S^m} (u_{i,j}^m + u_{j,i}^m) dV^m \quad (3)$$

In order to avoid any localization of micro damage on macro scale results, a non-local approach has to be considered as below [11]:

$$\dot{\sigma}_{ij}^D(X') = D_{ij} C_{ijkl}^M \dot{\epsilon}_{kl}^M(X') \quad (4)$$

where $\dot{\epsilon}_{kl}^M$ is macro-strain, C_{ijkl}^M is fourth order elasticity stiffness tensor and D_{ij} can be obtained as follows:

$$D_{ij} = 1 - \hat{\sigma}_{ij}^t(X') [\hat{\sigma}_{ij}^e(X')]^{-1} \quad (5)$$

$\hat{\sigma}_{ij}^t(X')$ is average stress which was already shown and $\hat{\sigma}_{ij}^e(X')$ is elastic strain in the case of microdamage.

3. Results

In Fig. 2, the process of preparing RVE is shown. As it shows, the first step is clarifying the boundaries of grains via cad software, in the next step, image processing software was used in order to obtain the exact coordinates of grain automatically as well as separating grains. The benefit of this procedure is that the algorithm which was designed in this procedure is automatically able to propose exact information of every image which was abtained by SEM machines. So, boundary element method can be applied for huge ranges of SEM images without spending so much time.

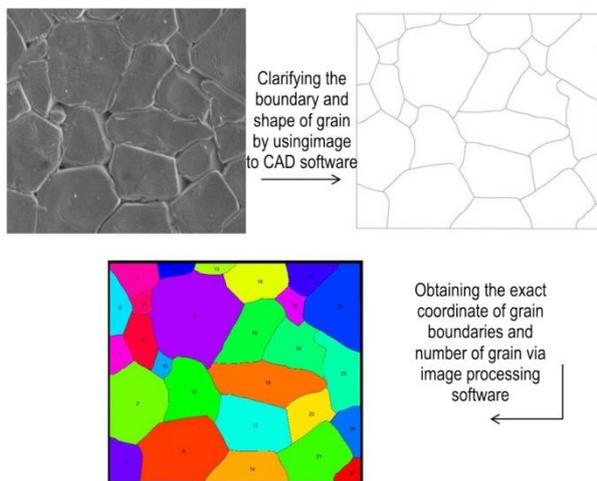


Figure 2. The workflow for generating the RVE of piezoelectric ceramics

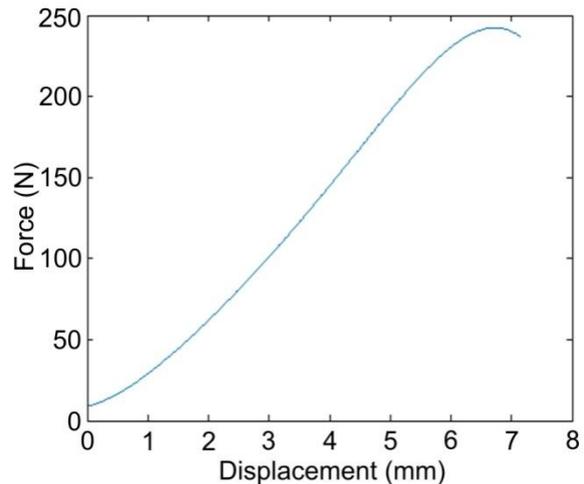


Figure 3. The reaction force versus displacement for the performed numerical simulations

Figs. 3 and 4 show the reaction forces and Potential jump for proposed grain. The reaction force can be obtained by multiplying average vertical stress on the length of that edge.

To study the influence of piezoelectric coupling on mechanical response, the calculations for two different cases with and without piezoelectric effect have been performed. The responses are

represented in Figure. 5. From the responses it can be concluded that, according to the numerical procedures, the maximum stress can be hardly influenced by the coupling between mechanical and electrical properties.

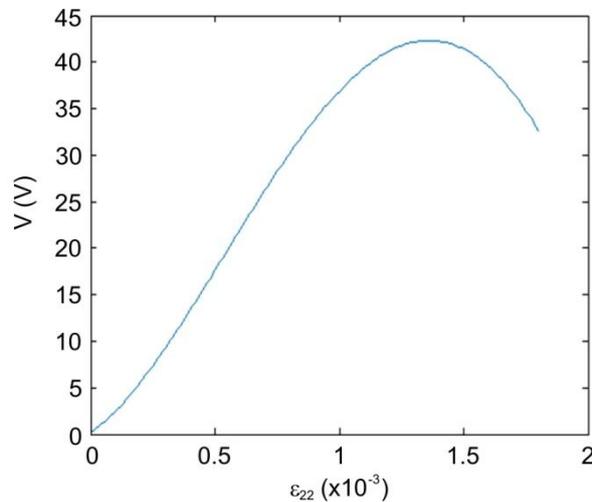


Figure 4. Potential jump V versus strain ϵ_{22} for the performed numerical simulations

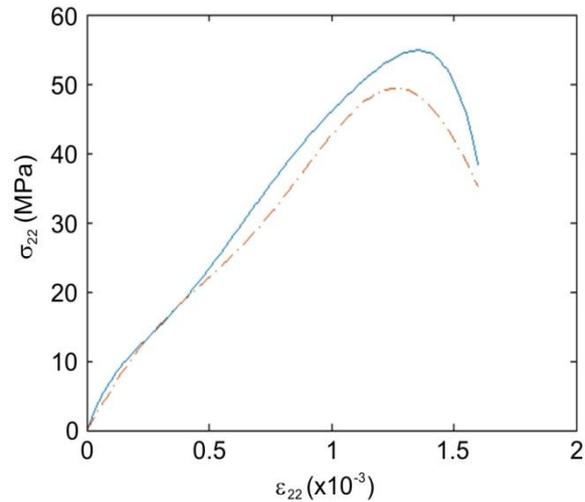


Figure 5. Stress σ_{22} versus strain ϵ_{22} for the simulations of polycrystal with (solid) and without (dashed) piezoelectric effect

4. Conclusions

In this study, the mechanical and electrical response of piezoelectric materials were investigated through multi scale boundary element methods. The algorithm which was designed by using image processing software allows one to study a huge ranges of SEM photo automatically. By using one of the photos which was gotten in laboratory via SEM machine, the numerical calculations have been done and the constitutive equations for polycrystalline materials were implemented into a boundary integral equation and the results and some examples were provided for piezoelectric ceramic.

Acknowledgments

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