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OPTIMIZATION OF CRYSTAL MICROSTRUCTURE IN PIEZOELECTRIC MATERIALS BY MULTISCALE FINITE ELEMENT ANALYSIS

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ABSTRACT

An increasingly higher performance is demanded of piezoelectric materials as they are applied to new technological fields such as MEMS / NEMS. Polycrystalline piezoelectric materials have a large possibility to exhibit higher performance in a macroscopic scale by design of crystal morphology in a microscopic scale. In this paper, a multi-scale finite element method by using crystallographic homogenization theory (Figure 1) has been applied to a typical piezoelectric material, barium titanate ($BaTiO_3$) in order to estimate macro homogenized properties considering crystal morphology in microstructure. Crystal orientations in microstructure has been then optimized by steepest decent method to maximize macro piezoelectric strain constants d_{333} and d_{311}, which are dominant factors for piezoelectric actuators.

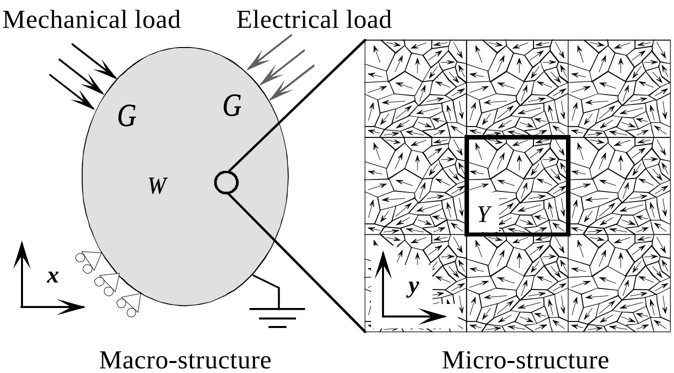
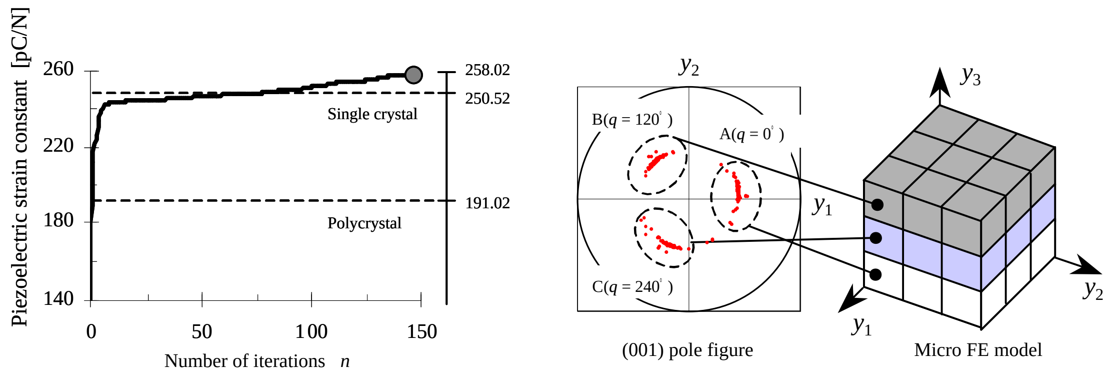


Figure 1 Macro- and micro-structures of polycrystalline piezoelectric materials.

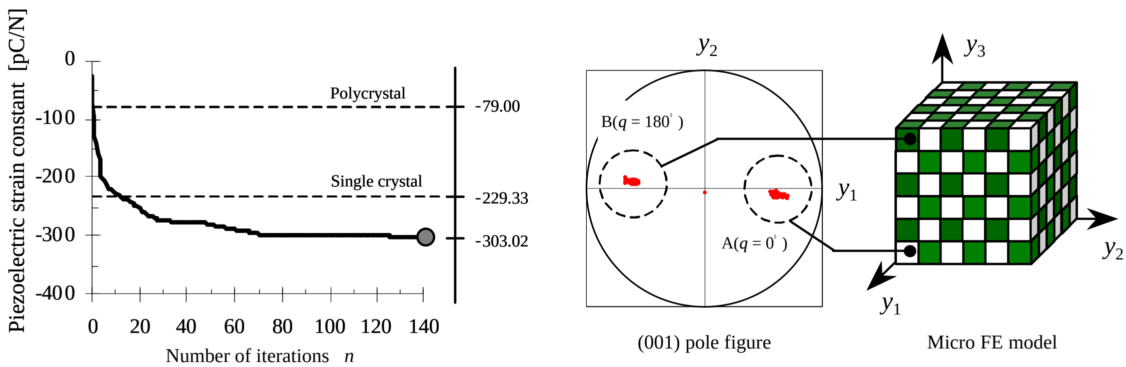
As computational results, two remarkable optimal solutions were obtained for microstructure. One is a polycrystalline structure found by setting macro piezoelectric strain constant d_{333} to objective function (Figure 2). It consists of three [111]-oriented crystals, which are in layers orderly with orientation gap 120 ° . If comparing with a conventional randomly-oriented polycrystal, the optimized microstructure presents

35 % increase of piezoelectric response. The other is a polycrystalline structure obtained for d_{311} (Figure 3). The optimized microstructure consists of adjacent crystals rotated by 180 ° in three dimensions, and it provides 284 % increase of piezoelectric response. In order to reveal the ideal crystal morphology for the largest piezoelectric strain constants, we analyzed the normal strains, e_{33} and e_{11} in microstructure when unit electric field was applied to macrostructure. Computations indicates that the normal strains in the both optimized microstructures becomes the largest by electrical and mechanical effects, and they lead to exhibit the highest piezoelectric response that is beyond single crystal.



(a) Macro piezoelectric strain constant (b) Microstructure

Figure 2 The optimized solution maximizing ${}^{macro}d_{333}$.



(a) Macro piezoelectric strain constant (b) Microstructure

Figure 3 The optimized solution maximizing ${}^{macro}d_{311}$.

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