

Computation of Piezo-electric Materials

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Piezo -electric materials are materials that will change its shape and size when an electric field is applied to the material. Vice versa, these materials will generate a certain voltage when they are bent, vibrated, or deformed. These materials show promising future, because they link mechanical and electrical properties of a material. In 21st century when electronic devices such as smart phones or touch-screen TV's depend highly on mechanical input such as human's touch, developing and researching materials that can link the mechanical and electrical properties can greatly improve the quality of i-phones. The main challenge regarding piezo-electric material research is predicting which microscopic and crystal structure will give the greatest piezo-electric property. There are infinite number of combinations possible in this world to create a piezo-electric material, and this paper focuses on accurately predicting these properties for a given microscopic structure. Manually experimenting and analyzing every combination of piezo-electric materials is laborious and time-consuming, so this paper introduces a computer-generated simulation program that will numerically compute the piezo-electric properties for various materials with different crystal structures. In this paper, two materials: barium Titante and PZT are used as sample materials and were compared to their experimental piezo-electric data.