Characterising fracture behaviour of flexoelectric solids using newly proposed numerically robust mixed FE

P. H. Serrao*, **S. Kozinov**

Chair of Continuum Mechanics, Ruhr-University Bochum
Universitätsstraße 150, Bochum, Germany
prince.serrao@rub.de

The size-dependent phenomenon of flexoelectricity is well-known due to its application in high-precision micro- and nano-scale MEMS. Flexoelectricity is the electromechanical coupling of strain gradients and electric field (direct flexoelectricity) or electric field gradients and mechanical strains (converse flexoelectricity). It can be observed not only in dielectrics with centrosymmetric unit cells but also in piezoelectric materials that already exhibit linear electromechanical coupling. Since flexoelectricity is associated with strain gradients that are inversely proportional to the length scale, the higher-order electromechanical coupling becomes dominant at smaller scales and often exceeds the influence of piezoelectricity. Simulation of flexoelectricity along with piezoelectricity demands fully coupled higher-order electromechanical formulations.

The fracture behavior of piezoelectric and, later on, ferroelectric materials has been intensively studied in the last decades. Recently, numerical modeling of fracture in polycrystalline ferroelectric ceramics under monotonic and cyclic electromechanical loading was performed [1]. For the numerical modeling of flexoelectricity, a second-order collocation-based mixed FEM was proposed [2] by the authors. Moreover, two new numerically robust mixed finite elements for the classical mixed FE were developed and implemented [3].

The newly proposed elements [3] are used for the fracture mechanics simulations in the current work. An edge-cracked aluminum nitride panel is modeled as a characteristic problem. The simulations go beyond conventional modeling of flexoelectricity in dielectric solids and primarily aimed at studying the mutual interaction of piezoelectricity and flexoelectricity. That is, the numerical simulations of an edge-cracked panel illustrate the influence of a higher-order electromechanical coupling contribution on piezoelectric solids.

It was found that the ”smoothening” effect of strain gradient elasticity (SGE) along with flexoelectricity results in a substantial reduction of the crack tip opening displacement (CTOD). In contrast, a sudden increase followed by a smooth drop of electric potential is observed along the crack face. The inclusion of piezoelectricity in flexoelectric simulations further reduces CTOD. Furthermore, a tremendous change in the profile of the generated electric potential is observed. When the higher-order electromechanical coupling is considered along with piezoelectricity, a contradictory or superimposed behavior of the electric potential profile is observed depending on the polarity of the piezoelectric material. The dominance of the gradient terms strongly influences the results in the vicinity of the crack tip. By varying the flexoelectric coefficients, the influence of flexoelectricity on the electric potential profile along the crack surface is additionally investigated. The present work demonstrates and explores the combined action of the piezo- and flexoelectric constituents and their influence on the fundamental fracture parameters in the context of the linear elastic fracture mechanics.

References

[1] S. Kozinov and M. Kuna, Simulation of fatigue damage in ferroelectric polycrystals under mechanical/electrical loading, *J Mech Phys Solids* 116 (2018) 150–170.

[2] K. Tannhäuser, P. H. Serrao and S. Kozinov, Second-Order Collocation-Based Mixed FEM for Flexoelectric Solids, *Solids*, Special Issue *”Recent Advance in Ferroelectric Composites”* 4 (1) (2023) 39–70.

[3] P. H. Serrao and S. Kozinov, Numerically robust C^0-continuous mixed FE for analyses of size-dependent flexoelectricity in piezoelectric solids (2023), *submitted*.