R-CURVE BEHAVIOR OF FERROELECTRICS: A SEMI-ANALYTICAL APPROACH

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Summary In the present work we study toughness variation of ferroelectric materials (PZT-5H) considering different scales for different poling and loading conditions. On the macro-scale we apply an extended theory of stresses at interfaces in dielectric solids. Further, on the micro-scale, nonlinear effects are introduced by applying the small scale switching approximation. The analysis is done considering the full anisotropy and electromechanical coupling of the material.

THEORETICAL FRAMEWORK

Due to the brittleness of ferroelectric materials fracture mechanical approaches are playing an essential role in the modern research. The strength of these materials, in terms of the critical stress intensity factors, is significantly determined by nonlinear ferroic effects arising on the microscopic scale. These effects are modelled by decomposing the strain ϵ_{ij} and electric displacement D_i additively into a linear piezoelectric part denoted with a superscript rev and a remanent strain $\Delta\epsilon_{ij}$ and remanent polarization ΔP_i emerging due to polarisation switching phenomena. The macroscopic constitutive law in a representative domain (RVE) is given by

$$\begin{aligned} \epsilon_{ij} - \Delta\epsilon_{ij} &= S_{ijkl}\sigma_{kl} + g_{kij}(D_k - \Delta P_k) && (1)\\ E_i &= -g_{ikl}\sigma_{kl} + \beta_{ik}(D_k - \Delta P_k). && (2) \end{aligned}$$

Here, ϵ_{ij}, σ_{ij}, E_i, D_k are respectively the components of the total strain, local stress tensor, electric field and electric displacement vector. S_{ijkl}, g_{ikl}, β_{ij} are the reduced elastic compliances, piezoelectric constants and the dielectric impermeability, respectively. The stresses σ_{ij} and electric displacement D_i are expressed in terms of the near-field solution. This means that the problem under consideration is in general an arbitrary crack. The crack tip loading $\mathrm{K}_L^{\text{tip}}$ is given by the superposition of the applied loads $\mathrm{K}_L^{\text{app}}$ and the loads induced due to polarisation switching $\Delta\mathrm{K}_L(\mathrm{K}_L^{\text{app}})$:

$$\mathrm{K}_L^{\text{tip}} = \mathrm{K}_L^{\text{app}} + \Delta\mathrm{K}_L(\mathrm{K}_L^{\text{app}}), \qquad \text{where} \quad \Delta\mathrm{K}_L = \int_{(A)} h_{LN,j}(r,\varphi)\Delta\Sigma_{Nj}\mathrm{d}A. \tag{3}$$

The subscript L like all capital indices ranges from 1 to 4 and represents the three mechanical and the dielectric crack opening modes. It is worth noting, that by contrast to the state-of-the-art, the calculations performed in this work are done using the full anisotropy of the material and piezoelectric weight functions h_{LN} that have been derived in [1]. $\Delta\Sigma_{Nj}$ is the irreversible, i.e. remanent part of the generalized stress tensor which is assumed to be homogeneous within the process zones. The global fracture criterion can be written as $\mathrm{K}_L^{\text{app}} \geq \mathrm{K}_{LC}$, where the subscript "$_C$" denotes the material-specific fracture toughness required for critical crack growth. It is therefore obvious that the fracture toughness is strongly modified by polarisation switching phenomena. On the other hand, in a recent work [2] it was shown, that for a more general crack model in piezoelectric materials which considers also the macroscopic electrostatic crack surface tractions σ_{22}^{C}, the effective stress intensity factor $\mathrm{K}_L^{\text{app}}$ is significantly modified. In the present work we calculate the relevant contributions to the effective fracture toughness coupling the macroscopic and microscopic scales and analyse the dependence on the external loads and the poling direction.

Within each domain (RVE) the polarisation vector $\mathbf{P}$ is assumed to switch as soon as mechanical and electrical energy reduction exceeds a critical energy barrier w_{crit}. The switching is interpreted as the rotation of the polarization vector around the out-of-plane axis, see Figure 1. The variant of the switching $\pm 90^\circ$ or 180° is determined by the switching criterion, such as

$$\sigma_{ij}(\epsilon_{ij}^{\text{rev}} + \Delta\epsilon_{ij}) + E_i(D_i^{\text{rev}} + \Delta P_i) \geq w_{\text{crit}}, \qquad \text{where} \qquad w_{\text{crit}}^{\pm 90^\circ} = \sqrt{2}E_C P^0, \quad w_{\text{crit}}^{180^\circ} = 2E_C P^0. \tag{4}$$

That is, the mechanical stresses and the electric field components are assumed to be known and are not modified by the switching events. The components of the remanent strain $\Delta\epsilon_{ij}$ and remanent polarisation ΔP_i within the local coordinate system (η,ξ) were introduced in [3]:

$$\Delta\bar{\epsilon}_{ij}(\pm 90^\circ) = \epsilon_D \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \Delta\bar{P}_k^{+90^\circ} = P^0 \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad \Delta\bar{P}_k^{-90^\circ} = P^0 \begin{pmatrix} -1 \\ -1 \end{pmatrix}, \quad \Delta\bar{P}_k^{180^\circ} = P^0 \begin{pmatrix} -2 \\ 0 \end{pmatrix}. \tag{5}$$

Note, there is no partial switching allowed. Once the polarisation switches, the irreversible strain is locked and cannot be reverse-switched.

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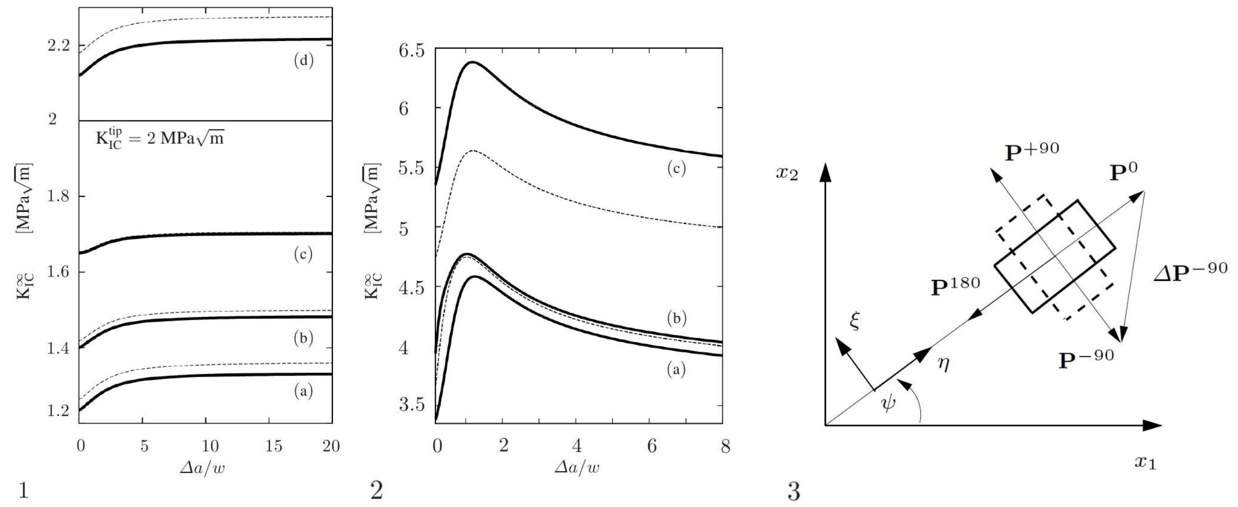

Figure 1: R-curves for mode-I stress intensity factor of PZT-5H with poling (1) perpendicular and (2) parallel to the crack faces and combined electromechanical loading. Solid curves represent the impermeable crack model and dashed curves stand for the semipermeable crack model including crack surface tractions, see [2]. The electrical loads are: (a) $K_{IV}^{\infty} = 0\cdot K_{IV}^{C}$, (b) $K_{IV}^{\infty} = 0.1\cdot K_{IV}^{C}$ (left), $K_{IV}^{\infty} = 0.3\cdot K_{IV}^{C}$ (right), (c) $K_{IV}^{\infty} = 0.3\cdot K_{IV}^{C}$ (left), $K_{IV}^{\infty} = 0.6\cdot K_{IV}^{C}$ (right) and (d) $K_{IV}^{\infty} = 1.25\cdot K_{IV}^{C}$. Sketch (3) shows three possible switching events of a tetragonal crystal unit cell in a plane.

RESULTS

We consider two important poling directions: poling perpendicular (x_2-direction) and parallel (x_1-direction) to the crack faces. Further, the intrinsic fracture toughness K_{IC}^{tip} is assumed to be $2\,\mathrm{MPa}\sqrt{\mathrm{m}}$ which is a typical value for the ferroelectric materials. The crack length is 5 mm. It should be noted that all calculations were iterated until Eq. (3) and the electrostatic boundary conditions at the crack faces were satisfied. The obtained R-curves are ploted in Figure 1. The plots show the effective mode-I fracture toughness as a function of the normalized crack extension for an electromechanical loading perpendicular to the crack faces. The electrical loads are given in terms of $K_{IV}^{C} = \sqrt{\pi a}\cdot\kappa E_C$ for demonstration purpose, with E_C being the coercive field and κ the corresponding dielectric constant of the material. As shown in Eq. (4) we consider on the micro-scale three different switching variants which results in three contributions to the effective fracture toughness,

$$\Delta K_L = \Delta K_L^{+90^\circ} + \Delta K_L^{-90^\circ} + \Delta K_L^{180^\circ}. \tag{6}$$

As expected, electrical loads increase the fracture toughness for both poling directions x_1 and x_2. Further, on the macro-scale two different crack models are analysed: the solid curves represent the impermeable model with $K_L^{app} = K_L^{\infty}$ and the dashed curves represent the semipermeable model with $K_L^{app} = K_L^{\infty} - K_L^{C}$, where K_L^{∞} are the external loads and K_L^{C} represent electrostaticaly induced crack surface tractions, see [3, 2]. For small electrical loads both models produce similar results. However, the difference becomes larger with increasing electrical loads. It is obvious that the reason for this is due to the different effective loads K_L^{app}. For poling perpendicular to the crack faces applying the semipermeable crack model results in larger toughness than for the impermeable crack model. In contrast, for poling parallel to the crack faces the effect is opposite. In this case the toughness is lowered by a significant amount.

CONCLUSIONS

In the present work we calculated the R-curves of ferroelectric materials such as PZT-5H considering effects on microscopic and macroscopic length scales, the full anisotropy of the material and the piezoelectric weight functions. On the macro-scale we applied two different crack models: impermeable and semipermeable. As expected, the fracture toughness is strongly modified by the switching phenomena. Further, the electrical loads play an essential role in toughness variation. The toughness increases with increasing electrical loads for both poling directions. The difference between the impermeable and semipermeable crack models varies with electrical loads and poling directions. In conclusion, one can state that an electrical field shields the crack tip which increases the fracture toughness with increasing field strength.

References

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