Technische Universität Bergakademie Freiberg
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Documentation

Implementing User Element for Phase field simulations of polarization switching-induced toughening in ferroelectric ceramics

06. October 2019

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2.1 Strong Form

An electrical enthalpy equation for ferroelectric system is a function of polarization P_i, strain ε_{ij} and electric field E_i as given below

$$h(P_i, \varepsilon_{ij}, E_i) = \alpha_i P_i^2 + \alpha_{ij} P_i^2 P_j^2 + \alpha_{ijk} P_i^2 P_j^2 P_k^2 + \frac{1}{2} c_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - q_{ijkl} \varepsilon_{ij} P_k P_l + \frac{1}{2} g_{ijkl} (\frac{\partial P_i}{\partial x_j}) * (\frac{\partial P_k}{\partial x_l}) - \frac{1}{2} k_0 E_i E_i - E_i P_i \quad (1)$$

From electrical enthalpy, the stresses and electrical displacements can be derived as

$$\sigma_{ij} = \frac{\partial h}{\partial \varepsilon_{ij}} \quad (2)$$

$$D_i = -\frac{\partial h}{\partial E_i} \quad (3)$$

2.2 Weak Form

Using principle of virtual work the weak form of governing equation can be written as

$$\int_V [\frac{\partial h}{\partial \varepsilon_{ij}} \delta \varepsilon_{ij} + \frac{\partial h}{\partial E_i} \delta E_i + [\frac{\partial h}{\partial P_i} + \frac{\partial}{\partial x_j} (\frac{\partial h}{\partial P_{i,j}})] \delta P_i]_{ij} dv = \int_S [t_i \delta u_i - \omega \delta \Phi + (\frac{\partial h}{\partial P_{i,j}} n_j) \delta P_i] dA \quad (4)$$

t_i= surface traction ω =surface charge $\frac{\partial h}{\partial P_{i,j}} n_j$ = surface gradient flux
writing $P_{i,j} = \xi_{ij}$ and $\frac{\partial h}{\partial P_{i,j}} n_j = \pi_i$ equation 4 becomes

$$\int_V [\frac{\partial h}{\partial \varepsilon_{ij}} \delta \varepsilon_{ij} + \frac{\partial h}{\partial E_i} \delta E_i + \frac{\partial h}{\partial \xi_{ij}} \delta \xi_{ij} + \frac{\partial h}{\partial P_i} \delta P_i] dV = \int_S [t_i \delta u_i - \omega \delta \Phi + \pi_i \delta P_i] dA \quad (5)$$

2.3 Weak form in matrix form

Equation 5 can be expressed in the matrix form as:

An 8 node brick element with seven degrees of freedom is considered (3 displacement components, 1 electrical potential and 3 polarization components)

Displacement, Electrical potential and Polarization can be expressed by the values at nodes, I, as

$$u = [N_u]\{u^I\}, \phi = < N_\phi > \{\phi^I\}, P = [N_p]\{P^I\} \quad (6)$$

$[N_u], < N_\phi >, [N_p]$ are interpolation or shape functions.

The strains, Electric fields and polarization gradients can be expressed as:

$$\varepsilon = [B_u]\{u^I\}, E = -[B_\phi]\{\phi^I\}, \xi = [B_p]\{P^I\} \quad (7)$$

The Surface traction, surface flux and surface gradient flux are expressed as

$$T = [N_T]\{T^I\}, \omega = < N_\omega > \{\omega^I\}, \pi = [N_\pi]\{\pi^I\} \quad (8)$$

Substituting equations x and y in z results in residual equations as below

$$K_{uu} u_I - K_{uP} P_I - F_S = 0 - K_{\phi\phi} \phi_I + K_{\phi P} P_I - Q_S = 0 - K_{Pu} u_I + K_{P\phi} \phi_I + K_{PP} + K'_{PP} P_I - \Pi_s = 0 \quad (9)$$

Where $[K_{uu}] = \int_v [B_u]^T [c] [B_u] dV$

$[K_{uP}] = \int_v [B_u]^T [Q(P_i)] [N_P] dV$

$[K_{Pu}] = \int_v [N_P]^T [Q^i(P_i)] [B_u] dV$

$[K_{\phi\phi}] = \int_v [B_\phi]^T [\kappa_0] [B_\phi] dV$

$$[K_{\phi P}] = \int_v [B_\phi]^T [N_P] dV$$

$$[K_{P\phi}] = \int_v [N_P]^T [B_\phi] dV$$

$$[K_{PP}] = \int_v [B_P]^T [G][B_P] dV$$

$$[K'_{PP}] = \int_v [N_P]^T [\alpha(P_i)][N_P] dV$$

$$[F_S] = \int_S [N_u]^T [N_T] dS T_I$$

$$[Q_S] = -\int_S [N_\phi]^T < N_\omega > dS \omega_I$$

$$[\Pi_S] = \int_S [N_P]^T [N_\phi] dS \phi_I$$