Nonlinear bilateral caloric–electromechanical couplings in polycrystalline ferroelectrics

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This research is about irreversible domain wall motion leading to a temperature change of the material. The materials are mostly subjected to high frequencies and large electrical loads, which is why insufficient heat dissipation can lead to undesirable temperature developments, so-called self-heating. Predictions concerning polycrystalline material behavior are made by the condensed method.

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1 Introduction

Ferroelectric materials, such as lead zirconate titanate (PZT) or barium titanate (BT) are technically attractive ceramics because of their special properties. They are often used for actuators or sensors in the precision range. Problems arise due to irreversible domain wall motion leading to self-heating associated with changes in the material properties, thermal stresses and sometimes even phase transformations, whereupon the devices finally are inoperative. In low Curie temperature materials, such as BT, even depolarization is possible.

The aim of this work is to extend the so-called condensed method (CM), which was developed to calculate e.g. hysteresis loops and residual stresses for polycrystalline materials where spatial discretization of the grain structure, to predict the temperature evolution in ferroelectric materials on the basis of a single polycrystalline material point. The CM is suitable for the efficient implementation of various constitutive behaviors, taking into account interactions between grains or different components of a material compound with low computational complexity and high numerical stability [1]. For this purpose, the CM is extended by the nonlinear bilateral caloric–electromechanical couplings. In addition, a comparison of the results by this work and those of the FEM according to [4] is presented. For verification, the theoretical results from the CM and FEM are compared to experimental results in [3].

2 Basic equations

In addition to the nonlinear constitutive equations of a thermoelectromechanical problem

\[
\sigma_{ij} = C_{ijkl} (\varepsilon_{kl} - \varepsilon_{kl}^{irr}) - e_{ijkl} E_{ij} - \beta_{ij} \theta, \quad (1)
\]

\[
D_i = e_{ijkl} (\varepsilon_{kl} - \varepsilon_{kl}^{irr}) + \kappa_{ij} E_{ij} + k_i \theta + \mu^{irr}, \quad (2)
\]

\[
s = \beta_{ij} (\varepsilon_{ij} - \varepsilon_{ij}^{irr}) + k_i E_i + \gamma \theta, \quad (3)
\]

where \(\sigma_{ij}\) describes the mechanical stress, \(D_i\) the electric displacement and \(s\) the specific entropy and the electromechanical balance laws \(\sigma_{ijkl} = 0\) and \(D_{ijkl} = 0\), an energy balance is required to compute the distribution of temperature change due to irreversible domain wall motions. The rate-dependant formulation emanates from the local form of the first law of thermodynamics and the Gibbs’ fundamental equation of the thermodynamical potential [4]:

\[
-\dot{q}_{ij}^A + \dot{\omega}^{diss} = T \dot{s}. \quad (4)
\]

While \(T\) is the absolute thermodynamic temperature, \(\theta = T - T_0\) denotes a temperature change.

3 Homogeneous distribution of temperature change

Inserting FOURIER’s law of heat conduction into \(\dot{q}_{ij}^A\) (note that the tensor of heat conduction \(\lambda_{ij}\) is assumed to be homogeneous in the body) in Eq. (4), the rate-dependant dissipative energy equation follows as

\[
\lambda_{ij} \theta_{ij} + \dot{\omega}^{diss} = T \dot{s}. \quad (5)
\]
Assuming a homogeneous distribution of temperature change $\theta$ in a material point, the gradient $\nabla \theta$, and thus the derivative $\nabla \theta_{ij}$ disappears. This simplifies the energy balance and it remains $\dot{\omega}^{\text{diss}} = T \dot{s}$. Inserting Eq. (3) and the leading order terms of the dissipative power $\dot{\omega}^{\text{diss}}$ and neglecting reversible contributions to heating or cooling yields

$$\sigma_{ij} \dot{\varepsilon}_{ij}^{\text{irr}} + E_i \dot{P}_{irr}^{i} = T \left( \beta_{ij} \dot{\varepsilon}_{ij}^{\text{irr}} - \beta_{ij} \dot{\varepsilon}_{ij}^{\text{irr}} + \dot{\varepsilon}_{i}^{\text{pol}} + \gamma \dot{\theta} \right) = -T \beta_{ij} \dot{\varepsilon}_{ij}^{\text{irr}} + T \gamma \dot{\theta}. \quad (6)$$

Replacing time derivatives by incremental changes in Eq. (6) and rewriting the energy balance within the context of the CM [1, 2], the macroscopic multi–grain formulation is obtained as

$$\bar{u} = \left( \langle \sigma_{ij} \Delta \varepsilon_{ij}^{\text{irr}} \rangle + E_i \langle \Delta P_{irr}^{i} \rangle + T \langle \beta_{ij} \Delta \varepsilon_{ij}^{\text{irr}} \rangle \right) \frac{1}{T(\gamma)}, \quad (7)$$

where angled brackets denote quantities averaged over $M$ grains of a representative volume element (RVE), i.e. $\langle \xi \rangle := \frac{1}{M} \sum_{m=1}^{M} \xi^m \quad \forall m \in M$.

4 Results and Conclusion

Figure 1 shows the electromechanical loading schemes for the numerical examples which are shown in Figure 2. Starting from equation (7), Figure 2 shows the results for the temperature development vs. load cycles compared to the experimental results and those of the FEM.

The result from the simulation of a polycrystal, solid blue line, is in a good agreement with the experimental result [3] and those obtained by the FEM [4]. Due to the lack of internal grain stresses, the heating of a single crystal is larger than that of a polycrystal. On the other hand, the temperature development is reduced by using displacement boundary conditions according to $u_{2 \text{ext}} = 0$, since it leads to increased residual stresses. Based on the assumptions of this model, a stationary state is not attained, resulting in a monotonously increasing heating. Taking into account the temperature–dependent material parameters, the temperature change in the material is aiming towards zero with increasing heating and disappears when reaching the Curie–temperature.

The results presented in this work show that the extended CM is able to estimate the temperature evolution as a result of irreversible domain wall motion. The deviation between CM and experiment and FEM for a larger number of load cycles is caused by the adiabatic boundary conditions. Here, heat dissipation has to be taken into account.

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