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Continuum thermodynamics of unusual domain evolution-induced toughening effect in nanocracked strontium titanate

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ABSTRACT

This work is concerned with the analysis of both unusual mechanical and electric behaviors of nanoscale pre-cracked incipient ferroelectric of $SrTiO_3$ at room temperature. A nonlinear thermodynamic model based on the Ginzburg-Landau theory is thus constructed and employed, which takes into account the appropriate mechanical boundary conditions, the electromechanical coupling between the polarization and the mechanical strain, and the self-strains of the ferroelastic and ferroelectric phase transformations. A large toughening effect is explored as a consequence of a softening nonlinear mechanical behavior, which characterizes for nanoscale $SrTiO_3$, despite of the brittleness of bulk $SrTiO_3$ ceramic. Depending upon applied strain, the large toughening and nonlinear mechanical behavior are attributed to unusual domain evolution of strain-induced polarization from the crack tip, in which a local-to-global transition of ferroelectric phase takes place from polarization vortex to hybrid structure of vortex and stripe domains, and finally to stripe domain structure with Néel type domain walls. Here, we also show the great importance of cross-coupling between the ferroelectric polarization and mechanical strain as it intrinsically leads to the local-to-global transition of ferroelectric phase. More interestingly, such cross-coupling additionally scatters the concentrated stress near the crack tip to Néel type domain walls. The present findings shed light on the crucial role of mechanical strain in controlling both the size and topology of polarization structures in nanoscale $SrTiO_3$. Our numerical results also provide an insight into the vital role of strain-induced polarization for the toughness and strength of $SrTiO_3$ material. Based on our study, the applicability of the present results to other incipient ferroelectrics such as $CaTiO_3$, $EuTiO_3$, and $KTaO_3$ with the same mechanism would be interesting and possible.

1. Introduction

Strontium titanate $SrTiO_3$ (STO) is well-known as an incipient ferroelectric in its pure and unstressed form down to absolute zero, where no spontaneous polarization appears, and thus distinguishes from the common ferroelectric systems.

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Nomenclature

a	crack length
c_{ij}	elastic constants
D_i	electrical displacement
E_i	electric field component
F	total free energy
f	total free energy density
$f_{\mathbf{elas}}(p_i,q_i,\varepsilon_{ij})$	elastic energy density
$f_{\mathbf{elec}}(p_i,E_i)$	electrostatic energy density
$f_{\mathbf{grad}}(p_i,q_i)$	gradient energy density
$f_{\mathbf{Land}}(p_i,q_i)$	landau energy density
G_p	gradient energy coefficients of polarization
G_q	gradient energy coefficients of structural order parameter
H	height of the model
K_I	mode-I stress intensity factor
L_p	kinetic coefficient related to polarization evolution
L_q	kinetic coefficient related to structural order parameter evolution
n_j	normal unit of surfaces
p_i	polarization
$p_{i,j}$	derivative of the *i*th component of the polarization vector pi with respect to the *j*th coordinate *xj*
q_i	structural order parameter
$q_{i,j} = \partial q_i/\partial j$	derivative of the *i*th component of the structural order parameter vector *qi* with respect to the *j*th coordinate *xj*
Q_{ij}	electrostrictive coefficients
r	spatial vector
t	time
T_C	curie temperature
t_i	surface traction
t_{ij}	coupling coefficients of $\boldsymbol{p}$ and $\boldsymbol{q}$
u_i	mechanical displacement
V	volume of the STO system
W	width of the model
xj	coordinate
α_i, α_{ij}	landau coefficients related to polarization
β_i, β_{ij}	landau coefficients related to structural order parameter
ε_{glob}	global applied strain
ε_{ij}	elastic strain
κ_c	dielectric constant of the background material
Λ_{ij}	linear-quadratic coupling coefficients between the structure order parameter and mechanical strain
σ_{ij}	stress
ϕ	electrostatic potential
ω	surface charge
STO	$SrTiO_3$
TDGL	Time-Dependent Ginburg-Landau equation

However, STO exhibits ferroelectricity at room temperature under substantial tensile strain [1–6]. Such gigantic enhancement in the ferroelectric transition temperature (T_C) under tensile strain that gives rise a distinct shift in properties had never been clearly seen in any ferroic system. However, this achievement was experimentally realized for the theoretical predictions [2], bringing about potential application for advanced devices [1,7,8]. The tensile strain magnitude that shifts the T_C of STO to the vicinity of room temperature is determined about 1% from both theoretical predictions and experimental observations [1–4]. According to the previous studies [1–6], the paraelectric-to-ferroelectric phase transition in STO thin film can take place due to the biaxial tensile or compressive in-plane strains provided by substrate. For the in-plane biaxial tensile and compressive strains, the polarization is in-plane and out-of-plane, respectively. In both strains, the polarization is parallel to the direction with the tensile deformation of lattice. The lattice deformation induced by the uniaxial tensile strain can be thus equivalent to that of biaxial compressive strains. As can be understood from Fig. 1, one-dimensional simplification structure of $SrTiO_3$ shows certain stable polarization values corresponding to a minimum energy based on the Landau theory under different levels of applied uniaxial tensile strain. Therefore, mechanical strain is a deceptively simple yet incisive means for unlocking emergent multifunctional properties in STO material and a promising way to minutely control ferroelectricity.

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