Ferroelectrics, 2001, Vol. 252, pp. 137-144
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The Structure of S-Walls in $m\bar{3}m \rightarrow mmm$ Ferroelastics

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(Received June 2, 2000)

The S-walls (also called W'-walls) refer to those domain walls whose orientations do not coincide with crystallographic planes but rather change with temperature. A simple continuum model has been constructed to describe the S-wall structures that occur at a $m\bar{3}m \rightarrow mmm$ ferroelastic phase transition. The model describes local values of the elastic strain components and the temperature dependence of the S-wall orientation. Distortions of unit cells across an S-wall was obtained numerically.

Keywords: S-walls; W'-walls; Landau-Ginzburg model; crystal symmetry; ferroelastics; domain walls

INTRODUCTION

The S-walls (also called W'-walls) occur in certain ferroic species [1,2,3] and generally do not coincide with crystallographic planes. The orientation of S-walls (SWs) in ferroelastics depends on the values of spontaneous strain, hence, will change with temperature.

Because the "strange" physical nature and the high application potential for these SW structures, there have been intense experimental studies on them and many interesting results have been obtained. For example, intersections between S-walls and W-walls in ferroelectric $KNbO_3$ [4], temperature induced SW switching in ferroelastic phases of

$NaNbO_3$ [5] and $AgNbO_3$ [6]. S-walls have also been observed in many other orthorhombic materials, such as $PbZrO_3$ [7], $PbHfO_3$ [8], $Pb(Zr_{1-x}Sn_x)O_3$ [9] and $Pb(Yb_{0.5}Nb_{0.5})O_3$ [10].

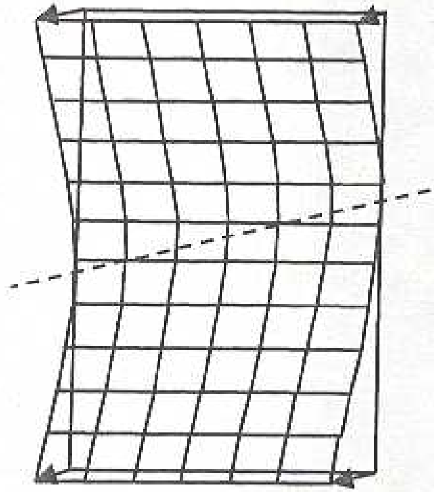

FIGURE 1. Distortion near the S-wall for $4/m \rightarrow 2/m$ phase transition[11].

One earlier work on the SW structure was done for a $4/m \rightarrow 2/m$ ferroelastic phase transition by using a two-dimensional continuum model [11]. More recently, high resolution transmission electron microscopy has been used to characterize the SWs in monoclinic $LaNbO_4$ ($4/m \rightarrow 2/m$ ferroelastics) [12].

In this paper, we present a simple continuum model for the S-walls resulting from an $m\bar{3}m \rightarrow mmm$ phase transition, and also provide numerical solutions for the S-wall structure and strain variations near the SWs.

THEORETICAL MODEL

The $m\bar{3}m \rightarrow mmm$ ferroelastic phase transition has a shear strain component as the order parameter; the other components of the elastic strain tensor serve as secondary order parameters.

We consider twin structure characterized by the following two spontaneous strains [3],

$$S^{(1)} = \begin{pmatrix} S_1 & S_6 & 0 \\ S_6 & S_2 & 0 \\ 0 & 0 & S_3 \end{pmatrix}, \quad S^{(2)} = \begin{pmatrix} S_3 & 0 & 0 \\ 0 & S_2 & -S_6 \\ 0 & -S_6 & S_1 \end{pmatrix} \tag{1a,b}$$

In order to match the elastic strain at the interface, the orientation of the domain wall plane will depend on the values of spontaneous strain according to the following relation

$$(S_1 - S_3)(x_1 - x_3) + 2S_6 x_2 = 0 \tag{2}$$

All strain components used here are expressed in the same cubic coordinate system of parent paraelastic phase.

Simplified free-energy density (invariant in $m\bar{3}m$) can be written as

$$\begin{aligned} F(\eta_{ij}, \eta_{ij,k}) = {} & \alpha_1(\eta_4^2 + \eta_5^2 + \eta_6^2) + (\eta_1^2 + \eta_2^2 + \eta_3^2) + \\ & \alpha_2\{\eta_1(\eta_5^2 + \eta_6^2 - 2\eta_4^2) + \eta_2(\eta_4^2 + \eta_6^2 - 2\eta_5^2) + \eta_3(\eta_4^2 + \eta_5^2 - 2\eta_6^2)\} \\ & \alpha_3(\eta_4^4 + \eta_5^4 + \eta_6^4) + g\{(\frac{\partial \eta_4}{\partial x_1})^2 + (\frac{\partial \eta_5}{\partial x_2})^2 + (\frac{\partial \eta_6}{\partial x_3})^2\}. \end{aligned} \tag{3}$$

The linear elastic strains, η_{ij}, are defined by the derivative of the elastic displacement $\boldsymbol{u}$

$$\eta_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{4}$$

and expressed using the Voigt notation $\eta_1 = \eta_{11}$, $\eta_2 = \eta_{22}$, $\eta_3 = \eta_{33}$, $\eta_4 = 2\eta_{23}$, $\eta_5 = 2\eta_{13}$, $\eta_6 = 2\eta_{12}$. All the expansion coefficients in Equation (3) are assumed to be temperature independent except $\alpha_1 = \alpha_0\,(T-T_0)$, with $\alpha_0 > 0$. In order to reduce the number of independent coefficients in the free energy expansion, we have normalized the free energy density by the coefficient of the second term.

SW problem is translationally invariant along the wall plane and hence all quantities characterizing the SW should depend on the distance from SW only. We choose a new coordinate system with one of the axes (x'_1) perpendicular to the SW, and the remaining two axes (x'_2, x'_3) parallel to the SW plane (Figure 2). Due to this choice the orientation of the coordinate system depends on the values of spontaneous strains, i.e. on temperature.

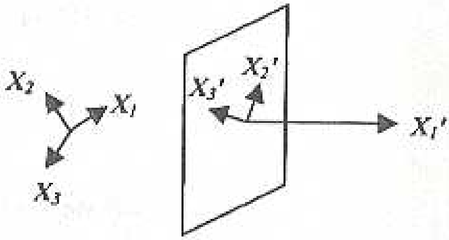

FIGURE 2. Relationship between the new and old coordinate systems.

The corresponding coordinate transformation can be chosen in a special form given by

$$\begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}C & \frac{1}{\sqrt{2}} & -D \\ \sqrt{2}D & 0 & C \\ -\frac{1}{\sqrt{2}}C & \frac{1}{\sqrt{2}} & D \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}, \tag{5}$$

$$C = \frac{S_1 - S_3}{\sqrt{(S_1 - S_3)^2 + 2S_6^2}}, \quad D = \frac{S_6}{\sqrt{(S_1 - S_3)^2 + 2S_6^2}} \tag{6a,b}$$

The components η_{ij} of the elastic strain in the free-energy must be transformed to the new coordinate system (denoted by a prime, $\eta'_1, \eta'_2, \eta'_3$, etc.).

S-WALL SOLUTIONS

The continuum SW solution can be derived from the Euler-Lagrange equations taking into account proper boundary conditions

$$\frac{\partial}{\partial x_k}\left[\frac{\partial F}{\partial \eta_{ij,k}}\right]-\frac{\partial F}{\partial \eta_{ij}}=0, \quad (i,j=1,2,3) \tag{7}$$

In materials without defects the following compatibility relations must also be satisfied [13]

$$\varepsilon_{ikl}\varepsilon_{jmn}\eta_{ln,km}=0, \quad (i,j,k,l,m,n=1,2,3) \tag{8}$$

where ε_{ijk} is the Levi-Civita's tensor (permutation symbol). Equations (7) and (8) are given in invariant tensor form, independent of the choice of the coordinate system. In the rotated coordinate system the compatibility relations are reduced to

$$\eta'_{22,11}=0, \qquad \eta'_{33,11}=0, \qquad \eta'_{23,11}=0 \tag{9}$$

because all strains depend on x'_1 only due to the translational symmetry.

In non-homogeneous system, five components of the spontaneous strain in Equation (1) (transformed to the rotated coordinates) are equal in both domains, but the shear strain component S'_6 (order parameter) has opposite signs in the two domains. The boundary conditions for the elastic strains should match spontaneous strains of domain 1 as $x'_1 \to +\infty$ and domain 2 as $x'_1 \to -\infty$

$$\lim_{x'_1\to\pm\infty}\eta'_\alpha(x'_1)=S'^{(1)}_\alpha, \ \lim_{x'_1\to\pm\infty}\eta'_6(x'_1)=\pm S'^{(1)}_6, (\alpha=1,2,...,5) \tag{10a,b}$$

The compatibility relations Equation (9) can be integrated and the strain tensor components parallel to the SW $(\eta'_2,\eta'_3,\eta'_4)$ must be constant due to the required boundary conditions Equation (10a). For convenience, we introduce the dimensionless strain components

$$y'_1=\frac{\eta'_1}{S'_1}, \quad y'_5=\frac{\eta'_5}{S'_5}, \quad y'_6=\frac{\eta'_6}{S'_6}.$$

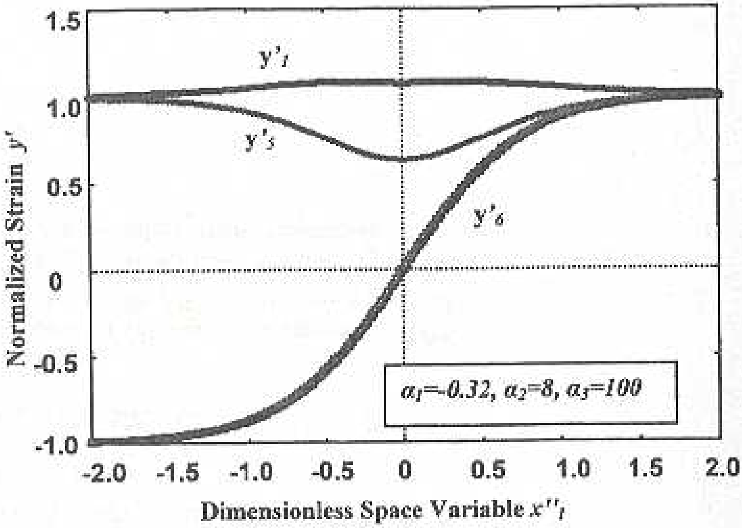

FIGURE 3. Normalized strain components across an S-wall at a specific temperature below T_0.

Finally, the SW problem reduces to solving the following three coupled differential equations (dimensionless coordinate $x_1^{''}$ is defined by $x_1^{''} = \frac{x_1^{'}}{\sqrt{g}}$)

$$\frac{d^2 y_\alpha^{'}}{dx''^2_1} = R_\alpha(y_1^{'}, y_5^{'}, y_6^{'}), \quad (\alpha = 1,5,6) \tag{11}$$

The functions R_1, R_5, R_6 are third-order polynomial functions in terms of the relative elastic strains y'_1, y'_5, and y'_6. The coefficient of each term is a complicated function of the coefficients α_1, α_2, and α_3 and will change with temperature. Typical solution of a twin with an SW is given in Figure 3.

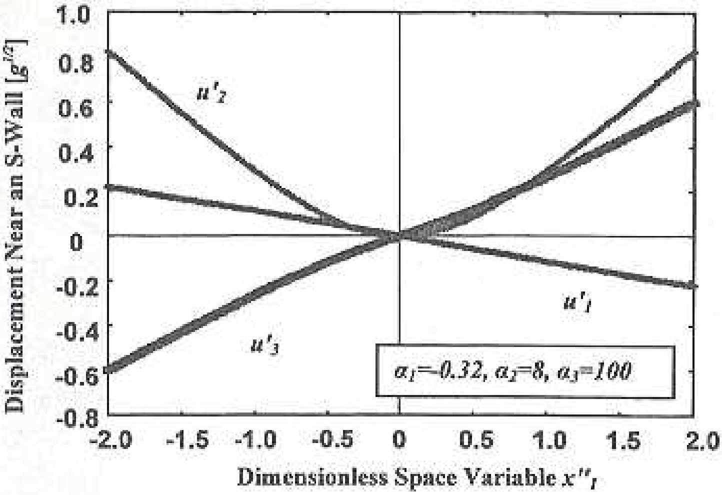

FIGURE 4. Displacement profile across an S-wall at a specific temperature below T_0.

The elastic displacements can be found by numerically integrating the corresponding strain components in rotated coordinates, i.e. Equation (4). Typical solutions of the elastic displacements are shown in Figure 4.

SUMMARY

A simple three-dimensional continuum model has been developed for the ferroelastic S-wall structure produced by a $m\bar{3}m \rightarrow mmm$ ferroelastic phase transition. The elastic strains as well as displacements near an S-wall have been calculated using this model. In general, lattice deformation near the S-wall not only contains longitudinal strain but also includes nonzero shear strain components. Although the SW solution is only numerical, our three-dimensional model provides a unique theoretical tool to study SW structure in the systems produced through a $m\bar{3}m \rightarrow mmm$ ferroelastic phase transition.

ACKNOWLEDGEMENTS

This work was supported by the NSF under grant number DNS 9704714 and the ONR under grant numbers N00014-98-1-0527 and N00014-96-1-1173. One of the authors (J.E.) is grateful for support from the Ministry of Education of the Czech Republic (J11/98:242200002) and from the Grant Agency of the Czech Republic (GAČR 202/00/1245).

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