Landau-Ginzburg Model of Interphase Boundaries in CsCl-Type Ferroelastics due to M-5 Mode Instability : LaAg1-xInx

D. Hatch, P. Hu, A. Saxena, G. Barsch

Landau-Ginzburg Model of Interphase Boundaries in CsCl-Type Ferroelastics due to M_5^- Mode Instability: LaAg$_{1-x}$In$_x$

D.M. Hatch, P. Hu, A. Saxena* and G.R. Barsch**

Department of Physics, Brigham Young University, Provo, Utah 84602, U.S.A.
* Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A.
** Materials Research Laboratory and Department of Physics, The Pennsylvania State University,
University Park, Pennsylvania 16802, U.S.A.

We have constructed a Landau-Ginzburg model of ferroelastic domain walls in the tetragonal phase of CsCl-type intermetallic compounds. This improper ferroelastic phase transition is driven by the condensation of a degenerate zone-edge phonon mode of M_5^- symmetry and can be described by a six-component order parameter. Analytic and numerical kink-type soliton solutions for the order parameter profile and the strain distribution are obtained for three different interphase boundaries: a twin boundary and two antiphase boundaries. The stability, merging and splitting of various domain types are also studied. Specifically, a symmetry-allowed product phase of I4/mmm (D_{4h}^{17}) symmetry has been experimentally observed in pseudobinary rare earth alloys of composition RAg$_{1-x}$ In$_x$ (R=La, Ce, Pr) and in related systems (YCu, LaCd).

I. INTRODUCTION

The study of various types of domain walls and their energetics in the context of both first and second order structural phase transitions has been carried out in recent years for ferromagnetic, ferroelectric and ferroelastic materials. Two kinds of domain walls, namely antiphase boundaries (APB) and twin boundaries (TB), occur in materials where the former are characterized by pure translations and the latter by rotations but not pure translations. Within the Landau-Ginzburg formalism a few analytic solutions for these domain walls can be obtained for relatively simple free energy functionals. However, it becomes an increasingly unwieldy task to classify and study all possible domain walls when (i) the primary and/or secondary order parameters are multi-component, (ii) there are several independent invariants in the gradient (Ginzburg) part of the free energy.

Here we identify possible interphase boundaries based on a systematic and comprehensive group theoretic treatment of domain walls using the concepts of the *direction* of the order parameter (OP) and the *isotropy group* of a domain class. For a given phase transition, this technique allows us to (a) construct all independent gradient invariants, (b) classify possible homogeneous phases, (c) classify all equivalent domains and domain pairs, (d) obtain criteria for the stability, merging and splitting of domain walls, (e) determine secondary OP and their effect on the domain walls, and finally (f) calculate the OP profile, domain wall energy and width. This technique has wide applicability in ferromagnetic, ferroelectric, ferroelastic, high T$_c$ superconductors (perovskites) and other materials.

We employ this technique for studying ferroic phase transitions occurring in materials with CsCl structure (space group O_h^1, Pm3m) induced by M_5^- mode softening, specifically a first order, improper ferroelastic transition to a tetragonally distorted low symmetry phase (D_{4h}^{17}, I4/mmm) in the pseudobinary rare earth alloy LaAg$_{1-x}$In$_x$ (x~0.2) [1]. The crystal structure is shown in Fig. 1. We have previously identified the six-component primary OP, nineteen secondary OP (including strain) and presented the Landau free energy (LFE) [2]. The class of OP directions consistent with the M_5^- irreducible representation and the observed atomic displacements is P$_{10}$ which has twelve equivalent directions (or domains) associated with it. In this work we find five gradient invariants. In the analysis of domain pairs we find only one class of twin boundaries, and two distinct classes of antiphase boundaries, denoted {1,2}, {1,4} and {1,10} respectively. Here the integers represent the selected directions (or domains) of the OP class P$_{10}$ and 1, 2, 4, and 10 denote {a,a,0,0,a,-a}, {0,0,a,-a,a,a}, {-a,-a,0,0,a,-a} and {-a,-a,0,0,-a,a}, respectively. The (soliton like) OP profiles, strains, stresses, energy, domain wall width are calculated and the constraints on the free energy coefficients are determined for each interphase boundary. Below we consider the {2,3} TB instead of {1,2} since the former is mathematically more convenient to analyze.

II. GINZBURG-LANDAU FREE ENERGY

The Ginzburg-Landau free energy (GLFE) for this transition is given by

$$F(\eta_i, \eta_{i,j}) = F_L(\eta_i) + F_G(\eta_{i,j}),$$

where $F_L(\eta_i)$ has been given to sixth order in η in Ref. [1]. Here $\eta = (\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6)$ is the six-component primary OP. In addition, F_{EL}, the invariants in strain (the secondary OP) and F_C, the coupling of strain with the primary OP, are given up to fourth order in Ref. [1]. In this work we also obtained five gradient invariants in $\eta_{i,m}$ from the symmetry of the primary OP and checked them against invariants generated by computer using the ISOTROPY program [3]:

$$F_G = D_1[\eta_{1,x}\eta_{2,x} - \eta_{1,z}\eta_{2,z} - \eta_{3,x}\eta_{4,x} + \eta_{3,y}\eta_{4,y} - \eta_{5,y}\eta_{6,y} + \eta_{5,z}\eta_{6,z}]$$

$$+D_2[\eta_{1,x}\eta_{2,z} - \eta_{1,z}\eta_{2,x} - \eta_{3,x}\eta_{4,y} + \eta_{3,y}\eta_{4,x} - \eta_{5,y}\eta_{6,z} + \eta_{5,z}\eta_{6,y}]$$

$$+D_3[(\eta_{1,y})^2 + (\eta_{2,y})^2 + (\eta_{3,z})^2 + (\eta_{4,z})^2 + (\eta_{5,x})^2 + (\eta_{6,x})^2]$$

$$+D_4[(\eta_{1,x})^2 + (\eta_{1,z})^2 + (\eta_{2,x})^2 + (\eta_{2,z})^2 + (\eta_{3,x})^2 + (\eta_{3,y})^2 + (\eta_{4,x})^2 + (\eta_{4,y})^2 + (\eta_{5,y})^2 + (\eta_{5,z})^2 + (\eta_{6,y})^2 + (\eta_{6,z})^2]$$

$$+D_5[\eta_{1,x}\eta_{1,z} - \eta_{2,x}\eta_{2,z} + \eta_{3,x}\eta_{3,y} - \eta_{4,x}\eta_{4,y} + \eta_{5,y}\eta_{5,z} + \eta_{6,y}\eta_{6,z}],$$

where $\eta_{i,m} = \frac{\partial \eta_i}{\partial m}$ (i=1,2,...6; m=x,y,z). Euler's equations lead to six coupled partial differential equations in η_i

$$\sum_m \frac{\partial}{\partial x_m}\left[\frac{\partial F}{\partial \eta_{i,m}}\right] - \frac{\partial F}{\partial \eta_i} = 0 ;$$

and three equations in stress

$$\sum_n \sigma_{mn,n} = 0,$$

where the stress is $\sigma_{ij} = \frac{\partial F}{\partial e_{ij}}$. In a homogeneous phase, the stress is zero everywhere, i.e. $\sigma_{ij} = 0$, from which we get $\frac{\partial F}{\partial e_l} = 0, l = 1, 2, ..., 6$ (using the contracted Voigt notation).

The OP gradient terms describe the generalized "exchange" interaction between neighboring domains in a material with spatially varying OP. The OP gradient coefficients for the GLFE pertaining to the above improper ferroelastic transition driven by the softening of the M_5^- mode can be determined from the dispersion of the phonon branches into which the soft mode frequency splits along the principal symmetry directions in the vicinity of the M point. We note that the gradient coefficients are related to the curvature of the phonon dispersion curves.

The same crystal structure can occur at several orientations relative to the parent phase. These domains correspond to various directions in the representation space. If the OP of one domain can be transformed by a group operation to that of another domain, these domains belong to the same class. From solutions for homogeneous phases we find the values of order parameters, which are then used as boundary conditions for the heterogeneous problems. We note that the elastic and coupling terms renormalize the coefficients of five fourth order invariants A_i to A_i' in the Landau free energy expression. This is consistent with the conclusion of the Landau theory that the symmetry of phases below T_c is entirely determined by the symmetry properties of the primary OP; i.e., the secondary OP's have no effect as far as crystal symmetry is concerned. The coefficient (k) of the second order invariant in LFE remains the same after the transformation. This verifies our procedure since it does not change the critical temperature T_c, which is determined by $k(T_c) = 0$. Compared to similar previous work [4] on phase transitions our free energy expression has the extra term of A_4'.

The primary OP that belongs to the minimum of the irreducible representation M_5^- as listed in the Tables by Stokes and Hatch [5]. For a domain of the P_{10} type we find that the free energy is,

$$F(P_{10}) = -\frac{k^2}{16A_1' + 8A_2' + 4A_3' - 4A_5'},$$

with $a = [-k/(16A_1' + 8A_2' + 4A_4' - 4A_4')]^{1/2}$. Since the free energy of a homogeneous stable domain or phase is generally negative (because lower symmetry domains are energetically more favorable than the higher symmetry phase), we assume that the denominator in the above equation is positive. For the domain P_{10} to be stable:

$$A_4' < 0, \quad A_4' - A_5' - A_3' > 0, \quad A_5' - A_4' + 2A_2' > 0, \quad A_3' - 3A_4' + 3A_5' - 4A_2' > 0, \quad 7A_5' - 2A_3' - A_4' > 0.$$

III. INTERPHASE BOUNDARIES

Any domain can be chosen as a representative for a given domain class. The group elements that do not change the order parameter of a domain form the *isotropy group*, F, of the domain. F must be a subgroup of G_0 (space group of the high symmetry phase). For the class of directions P_{10} the subgroup is D_{4h}^{17}. All domain pairs can be separated into *domain pair classes*. Domain pair classes can be determined by the decomposition of G_0 into *disjoint double cosets*: $G_0 = F^{(i)}eF^{(i)} + F^{(i)}t_{i,2}F^{(i)} + ... + F^{(i)}t_{i,r}F^{(i)}$. Each of the double cosets transforms domain P_i into P_r and determines the class of $(P(i), P(r))$. For the transition we are considering we obtain one twin boundary pair class, denoted $\{1,2\}$, and two distinct antiphase boundary pair classes, denoted $\{1,4\}$ and $\{1,10\}$.

Two ferroelastic domains can be distinguished by their spontaneous strains. In a ferroelastic crystal, the domain wall direction between two domains is along some specific direction. Assuming that in the domain wall the change of length of any infinitesimal vector due to the spontaneous strain should be the same for the two domains, i.e. $\tilde{x}(T - T')x = 0$, where T is the strain for one domain and T' is the strain for another domain. If a group operation A transforms one domain into another, then their tensors transform as follows: $\tilde{A}TA = T'$. Thus, for ferroelastic domains 1 and 2, we have the equation: $(a - b)(y^2 - z^2) = 0$. Then, $y = \pm z$ defines the domain wall for domains 1 and 2, i.e, for the domain pair $\{1,2\}$. A similar process leads to domain wall orientatins for the other domain pairs in this domain pair class.

We can also determine the conditions for *merging* and *splitting* of various domain walls, which are driven by the tendency of the system to achieve the minimum energy. In the merging or splitting relationships, the two pairs in each equation have one domain in common, and the two pairs meet by this common domain, i.e. $\{1,2\} + \{2,4\}$ is applicable to the following while $\{1,2\} + \{4,2\}$ and $\{1,3\} + \{2,4\}$ are not. $APB_1 + TB \rightarrow TB$, $APB_2 + TB \rightarrow TB$, $APB_2 + APB_2 \rightarrow APB_1$, $TB + TB \rightarrow TB$ and $APB_1 + APB_2 \rightarrow APB_2$. We have considered APB boundaries for the APB direction along a crystal axis and also at an angle θ to a crystal axis.

I. The $\{1,10\}$ antiphase boundary is formed between $D_1(\eta') = (\sqrt{2}a, 0, 0, 0, 0, \sqrt{2}a)$ and $D_{10}(\eta') = (-\sqrt{2}a, 0, 0, 0, 0, -\sqrt{2}a)$. New OP components have been defined where $\eta_1' = \sqrt{2}(\eta_1 + \eta_2), \eta_2' = \sqrt{2}(\eta_1 - \eta_2)$ etc. This antiphase boundary is formed by *half a lattice constant translation* of the lower symmetry phase along the z direction. The homogeneous solutions (homogeneous domains) serve as boundary conditions for heterogeneous solutions and thus $\eta' = \eta'(z)$. The common set $F^{(1,10)} = F^{(1)} \cap F^{(10)} = F^{(1)}$ keeps the domain pair invariant. The displacement pattern $\mathbf{d} = \{(a, a, 0), (-a, a, 0), (a, -a, 0), (-a, -a, 0)\}$ of the four Ag (In) atoms positioned at $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$, respectively is determined from the invariance under $F^{(1)} = D_{4h}^{17}$. Similarly, the displacement pattern for the center cubic La atoms positioned at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $(\frac{3}{2}, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{3}{2}, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, \frac{3}{2})$, respectively is found to be $\mathbf{d} = \{(0, 0, 2\alpha), (0, 0, 0), (0, 0, 0), (0, 0 - 2\alpha)\}$. For an antiphase domain wall to exist, the shears in the wall are generally zero, i.e. $\sigma_{31} = 0, \sigma_{32} = 0$. The strains, e_i's, satisfy *compatibility relationships* [6].

We get two coupled differential equations in η_1' and η_6'. For a *linear* type solution $(\eta_1' = \eta_6')$ we get

$$\eta_1' = \eta_6' = \tanh(\frac{z}{\xi_{APB}}), \quad \xi_{APB} = \sqrt{\frac{-2(2D_4 - D_1)}{K^+}},$$

where ξ_{APB} is the half width of the antiphase boundary and K^+ (and a, k' below) are algebraic combinations of A_i'. The strains e_1 and e_2 still keep the same values as that of the homogeneous phase and thus have no dependence on z. On the other hand, the strain e_3 in the direction perpendicular to the domain wall is dependent on position. We find that there is a *contraction* in the z direction $\Delta L_3 = \Delta u_3(+\infty) - \Delta u_3(-\infty)$ where $\Delta u_3(z) = u_3(z) - u_3^\infty$. The stress in the z direction σ_{33} is zero, which shows that we do not need to apply forces in the direction perpendicular to the domain wall, along which there is a contraction. However, $\sigma_{11} = \sigma_{22}$ are nonzero. Therefore, in an experiment to determine properties of such an antiphase domain wall, we need to apply forces parallel to, but no forces perpendicular to, the domain wall in order to maintain this structure. The domain wall energy, which we define as the thermodynamic potential difference of the crystal with a domain wall and the crystal in the homogeneous phase, is

$$E = \int_{-\infty}^{\infty} (F - F_0)dz = -\frac{4}{3}d_{APB}a^2k',$$

where $d_{APB} = 2\xi_{APB}$.

In the higher symmetry phase (in this case O_h^1), k is greater than zero. As temperature approaches the critical temperature T_c, k will approach zero. Thus, if $C_{11} > C_{12}$, then $k'/k < 0$. This implies that before the homogeneous phase transition, the *splitting* into different domains has begun. In the lower symmetry phase, $k < 0$. If $C_{11} < C_{12}$ and $3C_{11} > 2C_{12}$, then this antiphase domain structure will be stable. Otherwise, the antiphase structure will be unstable.
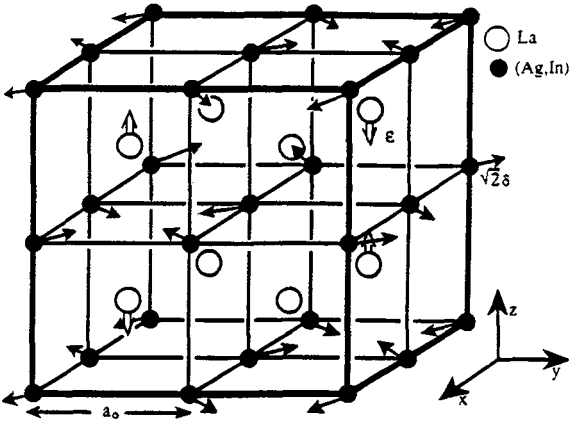
FIG. 1. Doubly-extended structure for the D_{4h}^{17} tetragonal low-temperature phase of LaAg$_{1-x}$In$_x$ with atomic displacements (After Ref. [1]).
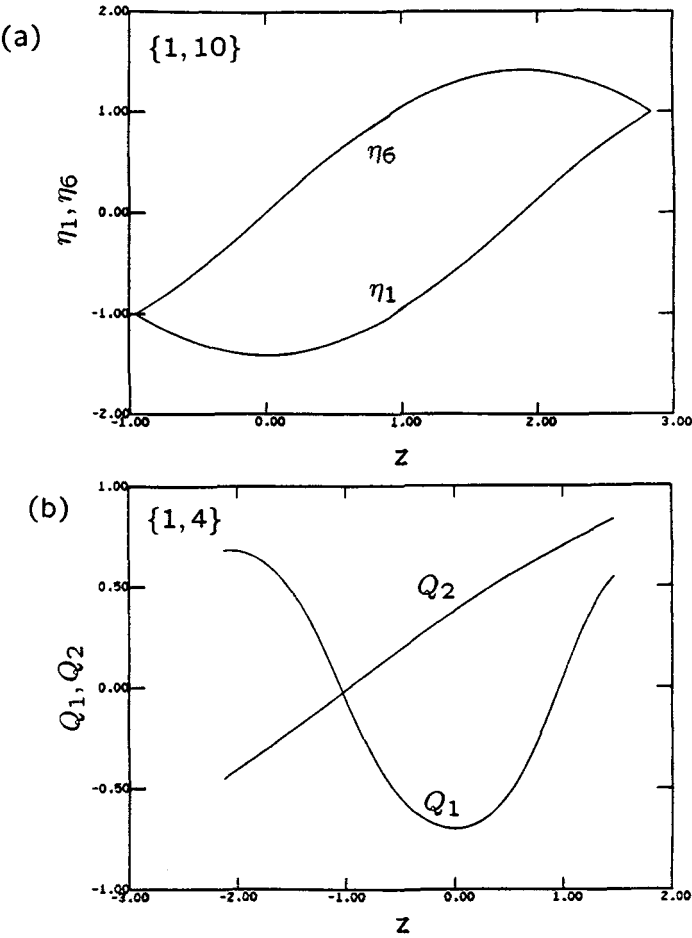

FIG. 2. Representative numerical solutions for kink-like domain walls for (a) $\{1, 10\}$ and (b) $\{1, 4\}$ antiphase boundaries.

We also explored the more general case by allowing the antiphase direction to form an angle θ with the crystal z axis. The coordinate transformation (with fixed origin) does not change η but the strains and gradient terms become a function of θ. From $\frac{\partial E}{\partial \theta} = 0$ we find that $\theta = 0°, 90°$ are solutions for stable configuarations.

The $\eta_2' = \eta_5' = 0$ and $\eta_1' = \eta_6'$ constitute a *linear* type of solution as obtained above. We also considered a *rotational* type of solution by setting $\eta_2' = \eta_5' = Q_1$, $\eta_1' = \eta_6' = Q_2$. The stability conditions for this linear type of solution are very specific. If these conditions are not satisfied, such as in the temperature range far from the critical temperature, the anti-ferroelastic components (η_2', η_5') will not be zero. Then we can get rotational solutions:

$$Q_1 = A \operatorname{sech}\left(\frac{x}{\xi_{APB}}\right), \quad Q_2 = \sqrt{2}a \tanh\left(\frac{x}{\xi_{APB}}\right),$$

$$A = \sqrt{\frac{2h_2 + 4h_5 a^2 y}{4h_3 y - 2h_5}}, \quad y = \frac{2D_4 - D_1}{2D_4 + D_1}, \quad \xi_{APB} = \sqrt{\frac{2D_4 + D_1}{2h_1 + 4h_5 a^2}},$$

where h_i are combinations of A_i' and elastic constants. However, this solution is stable under very *strict conditions*. Therefore, the assumption of linear solution above (η_2' and η_5' can be considered to be equal to zero) is likely to be true in most realized situations.

II. The **{1,4} antiphase boundary** is formed between $D_1(\eta) = (\sqrt{2}a, 0, 0, 0, 0, \sqrt{2}a)$ and $D_4(\eta) = (-\sqrt{2}a, 0, 0, 0, 0, \sqrt{2}a)$. This antiphase boundary is formed by *half a lattice constant translation* of the lower symmetry phase along the x direction. This domain pair is invariant under $F^{(1,4)} = F^{(1)} \cap F^{(4)}$. In domain 1, the displacements for individual atoms are: For La, $\mathbf{d} = \{(0, 0, 2\beta), (0, 0, 0,), (0, 0, 0), (0, 0, -2\beta)\}$ for atoms positioned at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), (\frac{3}{2}, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, \frac{3}{2}, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}, \frac{3}{2})$, respectively. For Ag(In), $\mathbf{d} = \{(\alpha, \alpha, 0), (-\alpha, \alpha, 0), (\alpha, -\alpha, 0), (-\alpha, -\alpha, 0)\}$ at position $(0, 0, 0), (1, 0, 0), (0, 1, 0), (0, 0, 1)$, respectively. Corresponding displacements in domain 4 are: For La, $\mathbf{d} = \{(0, 0, 0), (0, 0, 2\alpha), (0, 0, -2\alpha), (0, 0, 0)\}$ and for Ag(In), $\mathbf{d} = \{(-\alpha, \alpha, 0), (\alpha, \alpha, 0), (-\alpha, -\alpha, 0), (\alpha, -\alpha, 0)\}$. The domain wall is in the y-z plane.

By assuming $4A_1' + 4A_2' + 4A_5' = 0$, we find the following solution:

$$\eta_1' = \sqrt{2}a \tanh\left(\frac{x}{\xi_{APB}}\right), \quad \eta_6' = \sqrt{2}a, \quad \xi_{APB} = \sqrt{\frac{-2(2D_4 + D_1)}{k_1^+}}.$$

In addition we find that e_2, e_3 are constant, $\sigma_{12} = \sigma_{23} = \sigma_{13} = \sigma_{11} = 0$. The compressive stresses in the y and z direction are not equal. The domain wall energy is:

$$E = -\frac{2}{3}a^4 d_{APB}(-12A_1' - 8A_2' - 2A_3' + 8A_5').$$

A comparison of the energies $E_{1,10}$ and $2E_{1,4}$ shows that the positivity of the material dependent parameter $\alpha_1 - \alpha_2$ determines the stability relationship of domains. When $\alpha_1 > \alpha_2$, the domain pair $\{1, 10\}$ will split into two domains: $\{1, 10\} \rightarrow \{1, 4\} + \{4, 10\}$, otherwise $\{1, 10\} \leftarrow \{1, 4\} + \{4, 10\}$.

In the above solution we assumed η_6 to be constant while η_1 varied as a hyperbolic function. An alternative path between domains 1 and 4 is given by $\eta_1'^2 = \eta_6'^2$. Then, for $z > 0$ the solution is:

$$\eta_1' = \eta_6' = \sqrt{2}a \tanh\left(\frac{z}{\xi_{APB}}\right)$$

and for $z < 0$ we get $\eta_1' = -\eta_6'$. The only requirement for this solution is that the material dependent parameter $k_6^+/k_1^+ = 2D_3/(2D_4 + D_1)$. Which specific path will exist in a real crystal depends on the energies of various paths. We note that the criteria derived here for APB path vs. domain stability is an important feature of our analysis. We also considered an arbitrarily oriented domain wall between domains 1 and 4. We find that the strain remains the same as before the rotation, i.e. the x-y plane is homogeneous. The stable domain wall orientation is determined by $\partial E_{APB}/\partial \theta = 0$ which leads to $\sin 2\theta f(\theta) = 0$ and has solutions for θ distinct from the solution of $\sin 2\theta = 0$.

III. The **{2,3} twin boundary** is formed between $D_2(\eta') = (0, 0, 0, \sqrt{2}a, \sqrt{2}a, 0)$ and $D_3(\eta') = (0, \sqrt{2}a, \sqrt{2}a, 0, 0, 0)$. The domains 2 and 3 are related by a three-fold rotation along the (111) direction. In contrast to the antiphase pairs, twin domains are distinguished by their ferroic properties. Specifically, unlike APB pairs the two twin domains have *different* strains that can be detected optically. In domain 2, the displacement of the cubic center atom (La) is $\mathbf{d} = \{(0, 2a, 0), (0, 0, 0), (0, 0, 0), (0, -2a, 0)\}$ and in domain 3 the corresponding displacement is $\mathbf{d} = \{(2a, 0, 0), (0, 0, 0), (0, 0, 0), (-2a, 0, 0)\}$. The twin boundary has the following form: $\eta' = (0, \eta_2', \eta_3', \eta_4', \eta_5', 0)$ and

contains the x=y plane and the (110) direction. Since the shear strain is different in the two domains, the boundary conditions for shear strain are necessary.

For the special case $Q_1 = \eta_2' = \eta_3', \eta_4' = \eta_5' = Q_2$ we get two coupled differential equations. For the material dependent parameter $A_{1,2}^+ = 0$ (in a $45°$ rotated coordinate system r, s) we get

$$Q_1 = \frac{1}{\sqrt{2}}a[1 + \tanh(\frac{s}{\xi_{TB}})], \quad Q_2 = \frac{1}{\sqrt{2}}a[1 - \tanh(\frac{s}{\xi_{TB}})],$$

where $\xi_{TB} = \sqrt{-D^-/k_1^-}$. The domain wall energy is:

$$E = -\xi_{TB}(\frac{10}{3}k_1^- a^2 + \frac{8}{3}A_1^- a^4 + 2A_{1,2}^+ a^4),$$

where k_1^-, D^-, A_1^- and $A_{1,2}^+$ are material dependent parameters. The strains e_r', e_3' are constant and $\sigma_{ss} = 0$. The shear strain parallel to the domain wall is a function of position, but the shear stress is zero.

We can use the *initial value scan shooting method* to find solutions of two-variable coupled differential equations for the general problem of domain walls discussed above. The antiphase boundary $\{1,4\}$ has similar equations to those of the twin boundary $\{2,3\}$. The boundary conditions are also similar. Thus the general twin boundary case is covered by the antiphase pair $\{1,4\}$. The $\{1,10\}$ antiphase boundary case is considered separately. The stability conditions obtained above are borne out by the numerical solutions for linear vs. *disjunct* paths and also for the twin vs. *disjunct* paths. We show representative numerical solutions for the interphase boundaries in Fig. (2).

IV. CONCLUSION

We have employed powerful abstract group theoretical concepts to systematically describe antiphase and twin boundaries in a structural phase transformation, specifically in $LaAg_{1-x}In_x$. In particular, we decomposed the space group of the higher symmetry phase G_0 in terms of disjoint double cosets and utilized the concepts of equivalent domain pairs and the compatibility relations to find strains, stresses, width and energetics of the domain walls. We emphasize that group theoretical methods are systematic and have reduced our considerations to only three domain types represented by the domain pairs $\{1,4\}$, $\{1,10\}$ and $\{1,2\}$ rather than the 132 possible pairs that might initially be considered. Stability conditions were also obtained. Moreover, we determined mechanical stability of these interphase boundaries, namely contraction or rotation in the region of the domain wall, and the application of external lateral forces to sustain the structure in the crystal. Our technique is readily applicable to twin boundaries in high T_c superconductors [7], ferroelectrics, etc. The detailed study of the three domain pairs discussed above will be reported elsewhere [8].

V. ACKNOWLEDGMENTS

[1] J. Maetz, M. Müllner, H. Jex, W. Assmus and R. Takke, Z. Phys. B **37**, 39 (1980).
[2] A. Saxena, G. R. Barsch, and D. M. Hatch, Phase Trans. **46**, 89 (1994).
[3] H. T. Stokes and D. M. Hatch, unpublished.
[4] J. S. Kim, D. M. Hatch, and H. T. Stokes, Jap. J. Appl. Phys. **24**, 170 (1985).
[5] H. T. Stokes and D. M. Hatch, Isotropy Subgroups of the 230 Crystallographic Space Groups (World Scientific, Singapore, 1988).
[6] E. A. H. Love, A Treatise on the Mathematical Theory of Elasticity (Dover, New York, 1944), p. 49.
[7] Y. Zhu, A. R. Moodenbaugh, Z. X. Cai, J. Tafto, M. Suenaga, and D. O. Welch, Phys. Rev. Lett. **73**, 3026 (1994).
[8] P. Hu, D. M. Hatch, A. Saxena, and G. R. Barsch, to be submitted to Phys. Rev. B (unpublished).