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The zigzag interface shape at the ferroelastic phase transformation

Zdĕnek Kvítek†

Laboratoire de Spectrométrie Physique (Unité associée au CNRS 8), Université Joseph Fourier, BP 87, 38 402 Saint-Martin-d'Hères, France

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Abstract. The aim of this article is to analyse the shape of an interface between the paraelastic and ferroelastic phases in the static case when the sample is placed in a temperature gradient. It is shown that the resulting shape which is often of a zigzag form follows from the competition between the free energy induced by the gradient, the elastic-strain energy caused by lattice misfits along the interface and the interface surface energy. The evaluation of these energy contributions is unavoidable when their magnitudes are comparable.

In the first step we evaluate the change in elastic energy, which is due to the lattice misfit, for an anisotropic medium as the function of growth of the zigzag interface between the phases. In the second step we perform a complete analysis of the zigzag interface in the approximation of an isotropic medium.

As the main result of our analysis we show that the formation of a zigzag interface is energetically favourable when the ratio δ of the product of surface and chemical energies to the square of elastic-strain energy is small. When this condition is not satisfied, the interface remains flat. The analysis shows that depending on the value of δ a transition between the zigzag interface and the flat interface may exist which is discontinuous. This means that there exists a range of angles characterizing the zigzag shape which is forbidden.

1. Introduction

The shape of the interface between the paraelastic (prototype) and ferroelastic (product) phases has been studied for many years. The latter phase is often characterized by diffusionless atomic displacements; in macroscopic terms the transition is described by a spontaneous strain tensor \mathbf{u} . In this paper we discuss only first-order transitions with a discontinuous change in the spontaneous lattice strain \mathbf{u} . In addition, we shall have in mind cases where this change is large, as discussed below.

In the stationary case, the interface is formed so that the total energy is minimal. Nevertheless one kind of energy such as elastic-strain energy, surface energy or chemical free energy is often dominant. It is often the elastic-strain energy which plays the dominant role in determining the orientation of solid–solid interfaces. The simplest case is the discussion of the orientation of a planar interface; it is given by the minimum of elastic-strain energy caused by the elastic accommodation of lattice misfits. If lattice misfits disappear (strain-free interface), this elastic-strain energy is zero. This is the basic idea used by Fousek

† On leave from Institute of Physics, Na Slovance 2, 180 40 Praha 8, Czech Republic.

and Janovec (1969) and by Sapriel (1975) for the orientation of domain walls and by Boulesteix *et al* (1986) for interfaces between domains in paraelastic and ferroelastic phases, respectively, without volume changes. From the mathematical point of view it is possible to find this solution if one of principal values of spontaneous lattice strain \mathbf{u} is zero and two other principal values are of opposite signs. However, planar interfaces have been observed even for cases when the above-mentioned condition is not fulfilled. It was shown by Roitburd (1974, 1993) in a more general approach that one of the principal values of spontaneous strain \mathbf{u} may be only effectively equal to zero. He considers the ferroelastic phase as a conglomerate of twins (domains) in which the strains \mathbf{u} are different. The theory of Roitburd assumes that the polydomain structure is suitably modified in such a way that the tensor $\langle \mathbf{u} \rangle$ describing the average spontaneous strain in the ferroelastic phase is such that a planar interface can be formed. The ratio of volumes of the different twin components represents an additional free parameter which may make one principal value of the average spontaneous strain zero. This then determines the orientation of the planar phase interface.

Many interesting examples have been described in the review by Dec (1993).

Another approach was offered by Khachaturyan's (1967) theory, which is explained extensively in his book (Khachaturyan 1983). The theory concerns structural changes occurring between the paraelastic (prototype) phase and arbitrarily shaped inclusion of the ferroelastic (product) phase. The shape of the inclusion is controlled by the spontaneous strain tensor \mathbf{u} induced by the ferroelastic phase transformation. The interface can produce long-range forces which act in the bulk. The lattice misfits between prototype and product phases have to be compensated by elastic forces as long as other processes of elastic-strain relaxation such as the creation of dislocations or cracks do not occur. This theory is capable of determining the elastic-strain energy for an arbitrary homogeneous inclusion of the product phase precipitated in the infinite matrix of the prototype phase. The equilibrium of a two-phase system was studied by many workers see, e.g., Roitburd (1984, 1986) and Grienfel'd (1988) and it was demonstrated that these theories correspond to a partial case of the equilibrium between phases with a long-range interaction (e.g. electrostatic) governed by the same general description.

In the present contribution we shall study the solid–solid interface in an infinite sample placed in a temperature gradient field. From the thermal point of view the interface is forced to follow the isotherm with the temperature T_c characterizing the phase equilibrium without mechanical stress. The form of the isotherm is a plane perpendicular to the direction of the temperature gradient \mathbf{G} . However, the forces originating from the elastic-strain energy due to the lattice misfits cause the orientation of the interface to deviate from the orientation and position of the isotherm T_c . A zigzag-shaped interface is often observed in these cases for solid–solid interfaces. As an example, the zigzag shape of the phase interface observed between the ferroelastic–ferroelectric and paraelastic phases in KD_2PO_4 (DKDP) crystal (Bornarel and Cach 1994, Kvítek 1995) is shown in figure 1. This zigzag shape is conserved along the y axis (out of the page in figure 1).

Figure 1 shows the simplest situation with a symmetric zigzag interface which occurs when the direction corresponding to the highest modulus of the principal values of spontaneous strain (direction z in figure 1) lies in the plane of the isotherm. In addition, in this particular crystal all principal values are of the same sign. In this case, as is well known, the most favourable orientation of interface from the mechanical point of view is perpendicular to the direction of the highest modulus of the principal values of spontaneous strain.

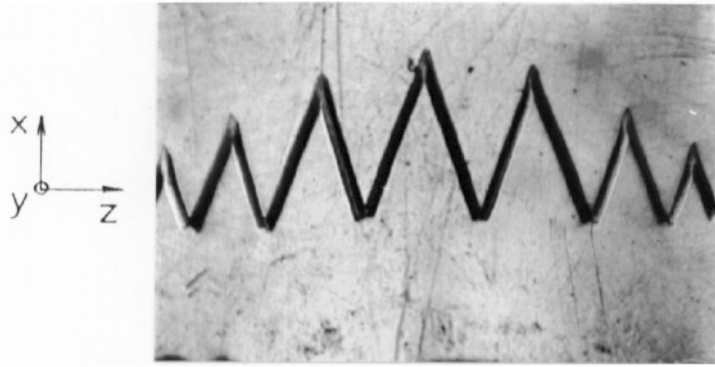


Figure 1. Photograph of the symmetric zigzag shape of the interface in a DKDP crystal between tetragonal and orthorhombic phases induced by the temperature gradient G oriented in the direction of the x axis.

2. Evaluation of energy density for a zigzag-shaped interface in an anisotropic medium

We model the interface (see figure 1) by an infinite periodic zigzag shape as shown in figure 2. All sections of the interface are considered to be parallel to the y axis. The plane of the drawing is determined by the z direction of the highest modulus of the principal values of spontaneous strain (in our case u_{zz}) and by the x direction parallel to the temperature gradient G . This approximation is valid in the middle of the crystal, where the relaxation of the stress on the facets is negligible and where the temperature distribution is defined by a constant temperature gradient with sufficient accuracy. We describe this symmetric zigzag formation by the angle β between the quasi-planar phase front parts and the x - y plane and the half-height e of the zigzag shape in the x direction, which are constant along the y direction.

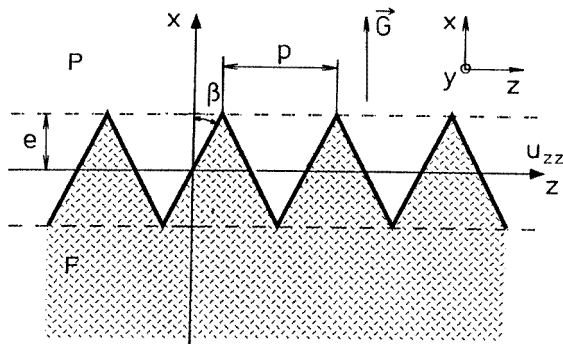


Figure 2. The symmetric zigzag shape of the interface between two phases distinguished by the spontaneous strain. The z direction is defined by the highest modulus of the principal values of spontaneous strain and the x direction parallel to the temperature gradient G .

For this reason we shall simplify our description to only the x - z plane; thus we shall investigate the total energy density ρ per unit length along z . The minimum of ρ as a function of two parameters β and e determines the shape of the symmetric zigzag interface.

This density is composed of three terms:

$$\rho = \rho_{elastic-strain} + \rho_{chemical} + \rho_{surface} \quad (1)$$

where $\rho_{elastic-strain}$ is the elastic-strain energy density, $\rho_{chemical}$ the chemical energy and $\rho_{surface}$ the energy density due to the surface of the phase front.

We shall now evaluate these terms for a zigzag-shaped interface described by the periodic function $\kappa(z) = \kappa(z + np)$ with n an integer, where the period

$$p = 4e \tan \beta$$

and by the shape on one period:

$$\kappa(z) = \begin{cases} e + \frac{z}{\tan \beta} \\ e - \frac{z}{\tan \beta} \end{cases} \quad \text{for } \begin{cases} p/2 < z < 0 \\ 0 < z < p/2. \end{cases}$$

2.1. Elastic-strain energy

We consider an infinite paraelastic (prototype) phase in which a ferroelastic (product) phase inclusion is precipitated characterized by a homogeneous spontaneous strain u_{ij} .

The elastic-strain energy of an arbitrarily shaped inclusion whose elastic moduli are identical with those of the matrix has the form (Khachaturyan 1983)

$$E = \frac{1}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} B(\mathbf{n}) |\tilde{\theta}(\mathbf{k})|^2. \quad (2)$$

Here

$$B(\mathbf{n}) = \lambda_{ijkl} u_{ij} u_{kl} - n_i \sigma_{ij} \Omega_{jl} \sigma_{lm} n_m$$

$$\sigma_{ij} = \lambda_{ijkl} u_{kl}$$

$$\Omega_{jl}^{-1} = \lambda_{qjlp} n_p n_q$$

$$\mathbf{n} = \frac{\mathbf{k}}{k}$$

where λ_{ijkl} is the component of the elastic modulus tensor and where

$$\tilde{\theta}(\mathbf{k}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \theta(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3r$$

represents the Fourier transformation of the function $\theta(\mathbf{r})$ which is equal to 1 inside and to 0 outside the inclusion. The first term $B(\mathbf{n})$ of equation (2) expresses the energy density of an infinitesimally thin plate-like inclusion and the function $|\tilde{\theta}(\mathbf{k})|^2$ describes only the inclusion shape of the ferroelastic (product) phase. $B(\mathbf{n})$ is a function only of the material parameters and of the orientation of the normal $\mathbf{n} = \mathbf{k}/k$ to the plate.

The elastic-strain energy associated with the zigzag interface (figure 2) is calculated using a special shape of the ferroelastic inclusion (figure 3) whose surfaces are modulated in the z direction by two adjacent zigzag interfaces characterized by the angle β and height $2e$. The volume of the inclusion is independent of these parameters. In what follows we shall always consider the inclusion volume per unit length along the y and z axes which is equal to h , the distance between adjacent interfaces. The artificial shape of the inclusion simplifies the calculation and causes no discrepancy in calculations of a single zigzag interface because there is no interaction between the adjacent surfaces as will be seen from the discussion of equation (3) for sufficiently large h ($h \geq 2e$).

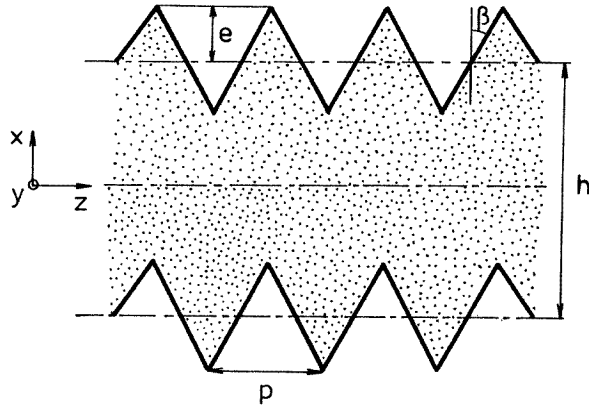


Figure 3. Shape of the ferroelastic (product) phase inclusion chosen for the modelled zigzag interface thickness h of this phase characterizing the 'volume' of this phase.

The density of the elastic-strain interface energy is given by (see appendix 1, equation (A1.6))

$$\rho(e, \beta)_{\text{front-elastic-strain}} = \frac{-A(\beta)2e}{12} + \frac{1}{4}hB(\beta' = 90^\circ) \quad A(\beta) > 0 \quad 0 < \beta < 90^\circ. \quad (3)$$

This expression shows that the shape of the interface described by parameters β and e is independent of the distance h because, after differentiation of the elastic-strain interface energy density with respect to β or e , the second term, which contains only the distance h , vanishes.

2.2. Chemical energy

For first-order transitions which we consider here, the change in $|\Delta F|$ in the chemical energy density with respect to its value at the temperature T_c is proportional to the local temperature $T(x) = G_x x$. The proportionality coefficient is equal to the jump $|\Delta S|$ in entropy at the transition:

$$|\Delta F| = |\Delta S||T(x) - T_c| = |\Delta S||G_x x|.$$

We recall that the value of T_c refers to zero stress. In figure 2 the isotherm of this temperature is placed in the middle of the zigzag interface and coincides with the z axis. For the chemical energy density per unit length of the zigzag structure along the z direction with the temperature gradient G_x parallel to the x axis, we obtain

$$\rho_{\text{chemical}} = \frac{4}{p} \int_0^{p/4} dz \int_0^{\kappa(z)} |\Delta S| G_x x \, dx = \frac{1}{6} G_x |\Delta S| e^2 \quad G_x > 0 \quad e > 0. \quad (4)$$

Our simplification of the problem consists in the fact that we consider separately the elastic-strain and chemical energies without any crossing term. From the viewpoint of symmetry the elastic-strain energy term reflects the symmetry of the crystal, while the chemical energy term corresponds to the symmetry of applied temperature gradient and we neglect the crossing term with product symmetry. This procedure is correct for a transition

of first order, in which case we can neglect, in the region of the zigzag examined, the temperature variation in spontaneous strain \mathbf{u} in comparison with the discontinuous change in \mathbf{u} during the phase transition. At the same time we assume a large jumpwise change in entropy during the transformation in the examined region. Consequently the modification of entropy by temperature or strain redistribution is neglected.

2.3. Surface energy

The additional contribution is due to short-range interactions between the phases, which can be represented by the surface energy. The surface area per unit length along the z direction increases with increasing angle β as $1/\sin \beta$. Hence the density of surface energy is equal to

$$\rho_{surface} = \frac{\gamma(\beta)}{\sin \beta}. \quad (5)$$

In fact it is difficult to measure or to estimate the value of the surface energy factor $\gamma(\beta)$ between two solid phases, which might be caused for example by anisotropy of chemical bonding. This factor could be interpreted in different ways. In a ferroelectric crystal such as DKDP, where the paraelastic–ferroelastic transition is coupled with the paraelectric–ferroelectric transition with one direction of spontaneous polarization \mathbf{P} , the surface energy is connected with the change in polarization near the interface. The surface energy factor $\gamma(\beta)$ is anisotropic. However, for small β this dependence is small compared with the contribution of the denominator in equation (5). This allows one to consider the surface energy factor as constant as it would be for an isotropic medium: $\gamma(\beta) = \gamma$. We take this approximation as valuable for the whole interval of β -values.

Instead of the surface energy we could also consider other contributions which would reduce the number of zigzag sections per unit length; this could be, for example, the energy of singularities, which are connected with the tips.

2.4. Density of total energy

Now we can write the density of total energy per unit length in the z direction, as a function of angles β and of the half-height e of the zigzag interface:

$$\Delta\rho(e, \beta) = \rho(e, \beta) - \rho(e = 0, \beta' = 90^\circ) = \frac{-A(\beta)2e}{12} + \frac{1}{6}G|\Delta S|e^2 + \left(\frac{1}{\sin \beta} - 1\right)\gamma. \quad (6)$$

This expression is defined in such a way that the energy of a flat interface with $\beta' = 90^\circ$ equals zero. The potential (6) is minimized for the following value of e :

$$e_{min} = \frac{A(\beta)}{2|\Delta S|G} \quad (7a)$$

at which the energy density takes the form

$$\Delta\rho(\beta) = \gamma \left[-\frac{[A(\beta)]^2}{24\gamma|\Delta S|G} + \left(\frac{1}{\sin \beta} - 1\right) \right]. \quad (7b)$$

3. Analysis of the zigzag-shaped interface for the simplified case of an isotropic medium

Equation (7b) is the consequence of a power e analysis of the energy terms mentioned above. We demonstrate the principal behaviour for the simplest situation with a single component u_{zz} of spontaneous strain perpendicular to the temperature gradient and the elastical modulus of crystal as approximated for an isotropic medium. These approximations give us a simple analytical expression for $A(\beta)$ (for details see appendix 2) (figure 4):

$$A(\beta) = \frac{2\mu}{1-\sigma}(1 - \sin^4 \beta)u_{zz}^2$$

$$\Delta\rho(\beta) = \gamma \left[-\frac{(1 - \sin^4 \beta)^2}{\delta} + \left(\frac{1}{\sin \beta} - 1 \right) \right] \quad (8)$$

where δ is given by

$$\delta = \frac{6}{u_{zz}^4} |\Delta S| G \gamma \left(\frac{1-\sigma}{\mu} \right)^2 > 0.$$

The character of the expression for $\Delta\rho(\beta)$ is governed by the sole parameter δ . It gives the ratio (without angular dependence) of the product of the surface energy and chemical energy to the square of the elastic-strain energy.

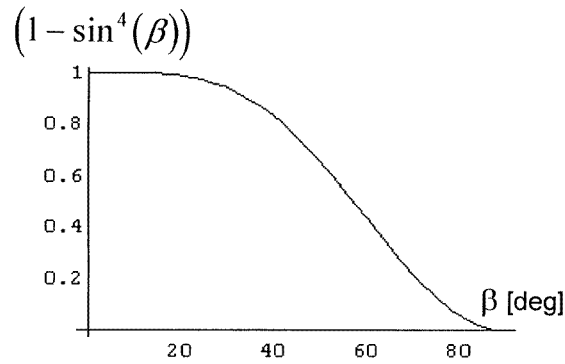


Figure 4. The factor $1 - \sin^4 \beta$ from the expression for $A(\beta)$ as a function of the angle β .

Figure 5 shows the form of the normalized energy density potential $\Delta\rho(\beta)/\gamma$ given by equation (8) for different parameters δ . The form of this potential shows that a flat interface with $\beta' = 90^\circ$ is stable for any value of the parameter δ . As long as

$$\delta \geq \delta_{crit} \approx 1.7 \quad (9)$$

this potential has only one minimum for a flat interface, as shown in figure 5(a).

When δ satisfies the inequality $\delta < \delta < \delta_{crit}$, the metastable minimum corresponding to the zigzag interface appears (figure 5(b)). This minimum becomes absolutely stable for δ in the interval $0 < \delta < \delta^0 \approx 1.4$ as shown in figure 5(c).

The extreme value of the potential occurs for the angle β_{min} defined by

$$\delta = 8(\sin^5 \beta_{min})[1 - (\sin^4 \beta_{min})] \quad (10)$$

and corresponds to a minimum for angles in the following interval:

$$0 < \beta_{min} < \beta_{crit} = \sin^{-1} \left(\left(\frac{5}{9} \right)^{1/4} \right) \approx 59.7^\circ.$$

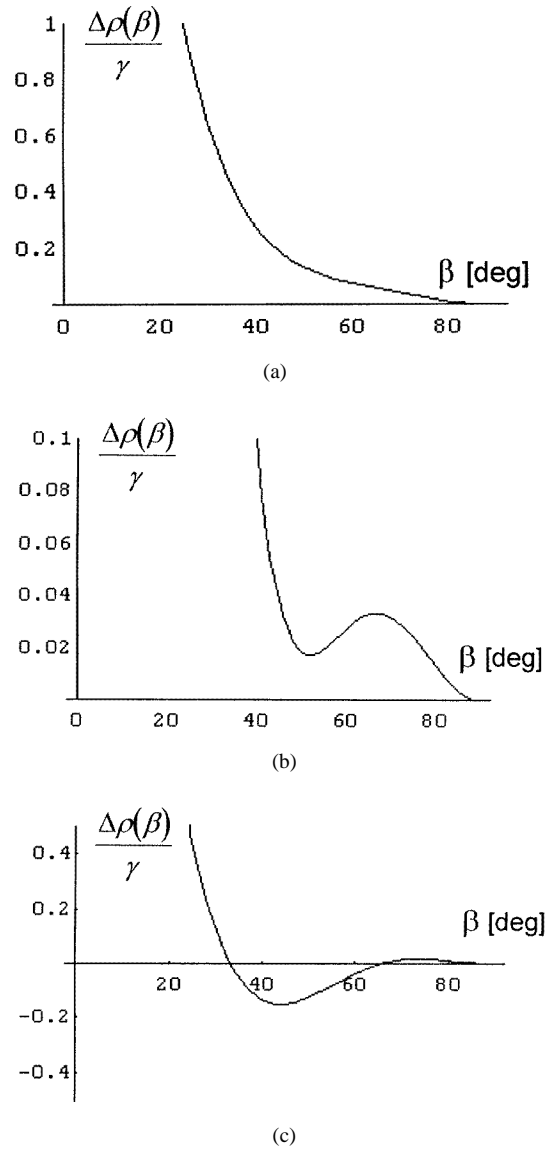


Figure 5. Variation in the normalized energy density with β for different values of the parameter δ in equation (8): (a) $\delta = 2.5$; (b) $\delta = 1.5$; (c) $\delta = 1.3$.

The inverse dependence of β_{min} as a function of δ is plotted in figure 6. The zigzag interface becomes absolutely stable for β_{min} smaller than $\beta^0 \approx 50.4^\circ$. The latter threshold value occurs for $\delta^0 \approx 1.4$ which has been calculated from equation (10) by substituting δ by δ^0 .

In figure 7 we present the value of the potential minimum as a function of β_{min} . The value of the density energy $\Delta\rho(\beta)$ corresponding to the flat interface $\beta = 90^\circ$ is constant and is defined zero by equation (8): for any value of δ while the energy value of the zigzag interface is δ dependent. The value of the potential minimum is negative, meaning that the

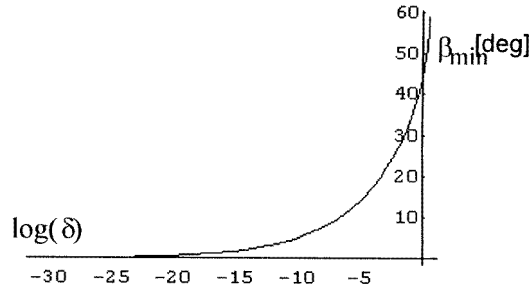


Figure 6. The angle β_{min} characterizing the position of minimum as a function of the parameter δ on a natural logarithmic scale.

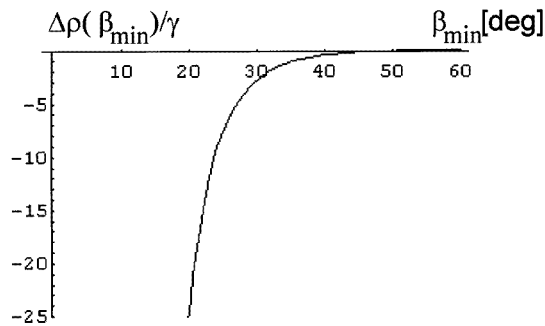


Figure 7. The normalized dependence of the potential minimum $\Delta\rho(\beta_{min})/\gamma$ as a function of β_{min} for the zigzag interface.

zigzag is absolutely stable for $\delta < \delta^0$ ($\beta_{min} \leq \beta^0 \approx 50.4^\circ$) and very deep for small δ as shown in figure 7.

A detailed discussion of metastability for $\delta < \delta < \delta_{crit}$ (figure 5(b)) is in reality worthless, because we cannot exclude the possibility that on the flat interface individual teeth of zigzag appear, forming no regular zigzag pattern. This process could proceed without hysteresis and is not included in the above theory.

4. Discussion

We have studied the shape of the interface by minimizing the total energy density composed of the elastic-strain energy due to lattice misfit between the phases, the chemical energy caused by the temperature gradient, and the interface energy proportional to the interface area. The choice of interface as an infinite periodic structure in the z direction (which lies in the plane of the isotherm of phase equilibrium without stress) is natural, because for an infinite crystal the interface cannot move far from the isotherm of phase equilibrium. The assumption of an infinite periodic interface allows us to use Fourier transformation simplifying calculations of elasticity based on the theory of Khachatryan. The application of this theory to the case of a zigzag interface shows that the density of energy is proportional to the height e of the zigzag structure. This result corresponds to the classical

approximate theories; one of them, Li (1972), describes the formation of a zigzag interface by decomposition of an edge quasi-dislocation characterizing lattice misfit into a dipole of disclinations. Alternative theories proposed by Roitburd (1988) and Marchenko (1981) are based on perturbation calculations.

All characteristic features of interface are demonstrated for the case of an isotropic medium. There exists one main parameter δ determining the existence of the zigzag interface. It has been found that only a flat interface is locally stable for any non-zero value of δ while the zigzag interface is stable only for the interval $0 < \delta < \delta_{crit}$. This interval determines the angles β_{min} : $0 < \beta_{min} < \beta_{crit} \approx 59.7^\circ$. The minimum energy of zigzag interface is always separated from the basic state energy characterizing a flat interface by a potential barrier. This means that the system needs some supplementary energy to change from one state to another. The results presented in figure 6 show that for small δ the angle β_{min} as a function of δ is almost constant. This means that the change in δ by many orders induces only small variations in β_{min} . Since the parameter δ is proportional to the modulus of the temperature gradient G , the variation in $|G|$ causes only tiny changes in the zigzag angle in comparison with the striking variations in the zigzag height $2e$ calculated using equation (7a).

We have demonstrated that for an interval of values δ ($\delta < \delta^0 \approx 1.4$) the formation of the zigzag structure is more favourable from the energy point of view than that of flat interface, as shown in figure 7. This condition is satisfied for example for the zigzag interface induced by a temperature gradient of the order of 1 K mm^{-1} in the crystal of DKDP shown in figure 1, where the angle β is approximately 22° . No angle greater than 25° was ever observed in the middle of crystal (Bornarel and Cach 1994, Kvítek 1995). A typical value of δ is 10^{-1} , which was determined using equation (8) and the following values: the entropy change $\Delta S = 17 \text{ kJ K}^{-1} \text{ m}^{-3}$ (Strukov 1972), and the isotropic approximation of elastic constants $\mu \approx 10^{10} \text{ J m}^{-3}$ and $\nu \approx 0.4$ was estimated from the Landolt-Börnstein (1982) tables. The highest strain in the z direction, $u_{zz} = 6.5 \times 10^{-4}$, was measured by Zeyen (1976) and for the surface energy we take the estimation $\gamma \approx 10^{-4} \text{ J m}^{-2}$ of Aleshko-Ozhevskij (1992) for the ferroelectric–paraelectric boundary in a DKDP crystal. The complete discussion of the DKDP case, including the anisotropy aspects and accounting for small positive estimated dilatation $u_{xx} = 10^{-4}$ in the x direction, will be given elsewhere. The precise measurement of this dilatation u_{xx} is very important for discussion of the DKDP crystal. If the contribution of small dilatation u_{xx} is of the same sign as u_{zz} , the position of modified potential minimum for $\beta_{min} = 0^\circ$ is conserved and the presented analysis is qualitatively still valid. On the other hand, if the signs of the dilatations u_{zz} and u_{xx} are not the same, for example in the case of a transition for which the volume is conserved, the orientation of the plane interface corresponding to minimum of elastic-strain potential would not be inclined with respect to the plane perpendicular to z axis and therefore the analysis presented above would not be applicable. The approach employed in this article can be used for any periodic shape of interfaces between two solid phases which may be anisotropic but whose elastic moduli have the same values. The solution presented applies to the solid–solid interface and, owing to an anisotropic mechanical strain field, is formally analogous to the interface analysis of liquid crystals presented in the book by de Gennes and Prost (1993). Many theoretical papers studying interfaces between a liquid and a uniaxially stressed solid have appeared recently (Nozieres 1991, 1993, Kassner and Mishbah 1994). These investigations were motivated by observation of the interface of ^4He (Balibar *et al* 1991). While this problem seems analogous to that treated in the present contribution, no zigzag shape has been observed in this case, probably because of the absence of the shear in liquid.

Acknowledgments

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Appendix 1

We calculate the density of elastic-strain energy per unit of length in the z direction induced by the zigzag interface in two dimensions (the x direction of the temperature gradient \mathbf{G} is perpendicular to the z direction of the highest modulus of the principal values of spontaneous strain \mathbf{u}):

$$\rho_{\text{elastic-strain}} = \frac{1}{2} \sum_m \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} B(\beta') |\tilde{\theta}_m(k_x)|^2$$

where the angle $\beta' = \tan^{-1}(k_x/k_z)$ describes the orientation of the vector \mathbf{k} and

$$\begin{aligned} \tilde{\theta}(\mathbf{k}) &= \tilde{\theta}\left(k_x, k_z = \frac{2\pi m}{p}\right) = \tilde{\theta}_m(k_x) \\ &= \frac{1}{p} \int_{-p/2}^{p/2} \exp\left(-i\frac{2\pi m z}{p}\right) dz \int_{\kappa(z)-h/2}^{\kappa(z)+h/2} \exp(-ik_x x) dx \\ &= \frac{1}{2} \frac{\sin(k_x h/2)}{k_x/2} \left\{ \frac{\sin(\pi m/2 + k_x e)}{\pi m/2 + k_x e} + (-1)^m \frac{\sin(\pi m/2 - k_x e)}{\pi m/2 - k_x e} \right\}. \end{aligned} \quad (\text{A1.1})$$

We can divide equation (A1.1) into the cases $m = 0$ and $m \neq 0$:

$$\tilde{\theta}_{m=0}(k_x) = h \frac{\sin(k_x h/2)}{k_x h/2} \frac{\sin(k_x e)}{(k_x e)} \quad (\text{A1.2a})$$

$$\tilde{\theta}_{m \neq 0}(k_x) = 2e \sin\left(\frac{k_x h}{2}\right) \frac{\sin(\pi m/2 + k_x e)}{(k_x e)^2 - (\pi m/2)^2}. \quad (\text{A1.2b})$$

Our task is to obtain the elastic-strain energy as a function of the height $2e$ of the zigzag and the angle β as parameters independent of the zigzag interface. If we suppose that the thickness h between horizontal interfaces is sufficiently large that we could neglect the mutual interaction between the zigzag interfaces, the density of elastic-strain energy of one zigzag interface is half the elastic-strain energy density:

$$\begin{aligned} \rho_{\text{front-elastic-strain}} &= \frac{1}{2} \rho_{\text{elastic-strain}} \\ \rho_{\text{front-elastic-strain}} &= \frac{1}{4} \left\{ \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} \sum_{m \neq 0} (-1) \left[B(\beta' = 90^\circ) |\tilde{\theta}_{m=0}(k_x)|^2 \right. \right. \\ &\quad \left. \left. - B\left(\beta' = \tan^{-1}\left(\frac{k_x}{k_z}\right)\right) |\tilde{\theta}_m(k_x)|^2 \right] \right\} + B(\beta' = 90^\circ) h. \end{aligned} \quad (\text{A1.3})$$

If we put the function $B = 1$, the integral is proportional to the ‘volume’ in \mathbf{k} space. This ‘volume’ in two dimensions per unit of length in the direction of the z axis is equal to h which is independent of the form of a zigzag:

$$h = \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} \left\{ B |\tilde{\theta}_{m=0}(k_x)|^2 + \sum_{m \neq 0} B |\tilde{\theta}_m(k_x)|^2 \right\} \quad (\text{A1.4})$$

with $B = 1$. The exact solution will be more evident if we eliminate the integral over the term $|\tilde{\theta}_{m=0}(k_x)|^2$ in equation (A1.3) by substitution from equation (A1.4):

$$\begin{aligned} \rho_{front-elastic-strain} &= \frac{1}{4} \left\{ \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} \sum_{m \neq 0} (-1) \left[B(\beta' = 90^\circ) |\tilde{\theta}_{m=0}(k_x)|^2 \right. \right. \\ &\quad \left. \left. - B \left(\beta' = \tan^{-1} \left(\frac{k_x}{k_z} \right) \right) |\tilde{\theta}_m(k_x)|^2 \right] \right\} + B(\beta' = 90^\circ)h \\ &= e \int_{-\infty}^{+\infty} d\xi \sum_{m \neq 0} -A(\beta') \sin^2 \left(\frac{\xi h}{2e} \right) \frac{\sin^2(\xi + \pi m/2)}{(\xi^2 - (\pi m/2)^2)^2} + \frac{1}{4} B(\beta' = 90^\circ)h \end{aligned} \quad (A1.5)$$

with

$$A(\beta') = B(\beta' = 90^\circ) - B \left(\beta' = \tan^{-1} \left(\frac{2\xi}{\pi m} \tan \beta \right) \right).$$

If we put $\beta' \rightarrow 0$ representing an interface flat in the direction of z axis, equation (A1.) approaches zero. The form of equation (A1.5) shows that the energy density of the arbitrary zigzag interface is proportional to its height e , because we can choose the ratio of h/e to be arbitrarily high. The exact solution of this problem requires numerical solution of equation (A1.5). Nevertheless, if we are looking for an approximate solution, we can simplify equation (A1.5) by supposing that the function A is smooth in comparison with the second multiplier in the integration. So we put the function A before the integration with angle $\beta' = \beta$ for which the second term of integration has its maximum. We are now able to evaluate the integrated value using the expression for $\tilde{\theta}_{m \neq 0}(k_x)$ from (A1.4):

$$\begin{aligned} \rho_{front-elastic-strain} &= \frac{1}{4} \left\{ (-1) A(\beta) \left[h - \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} |\tilde{\theta}_{m=0}(k_x)|^2 \right] + B(\beta' = 90^\circ)h \right\} \\ &= \frac{1}{4} \left\{ A(\beta) \left[\int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} h^2 \frac{\sin^2(k_x h/2)}{(k_x h/2)^2} \frac{\sin^2(k_x e)}{(k_x e)^2} \right] + B(\beta)h \right\} \\ &= \frac{1}{4} \left\{ A(\beta) \left[h - \frac{2e}{3} \right] + B(\beta)h \right\} = (-1) A(\beta) \frac{2e}{12} + \frac{1}{4} B(\beta' = 90^\circ)h. \end{aligned} \quad (A1.6)$$

Appendix 2

The elastic modulus tensor of an isotropic medium has the following non-vanishing components:

$$\begin{aligned} \lambda_{1111} = \lambda_{2222} = \lambda_{3333} = c_{33} &= 2\mu \frac{1 - \sigma}{1 - 2\sigma} \\ \lambda_{1122} = \lambda_{1133} = \lambda_{2233} = c_{13} &= 2\mu \frac{\sigma}{1 - 2\sigma} \\ \lambda_{1212} = \lambda_{1313} = \lambda_{2323} = c_{44} &= \mu \end{aligned} \quad (A2.1)$$

where μ is the shear modulus, σ is the Poisson ratio, and c_{11} , c_{13} and c_{44} are Voigt's designations where (x, y, z) is substituted by $(1, 2, 3)$. We consider only the non-zero component of strain in the direction of the z axis. The vector \mathbf{n} lies in the x - z plane with $n_1 = \sin \beta$ and $n_3 = \cos \beta$. Now we show how we can simplify equation (8) by rewriting equation (2) for an isotropic medium. The components of the elastic modulus must create stress with at least one index in the x - z plane (indices 1 or 3) which is at the same time

connected through the elastic modulus tensor with the sole component of the spontaneous strain, $u_{zz} = u_{33}$. Only two components take part: $c_{33} = \lambda_{3333}$, $c_{13} = \lambda_{1133}$.

After substitution we obtain the expression

$$B(n_1, n_3) = \lambda_{3333}u_{33}u_{33} - (n_3\lambda_{3333}u_{33})^2\Omega_{33} - 2n_1n_3\lambda_{1133}\lambda_{3333}u_{33}^2\Omega_{13} - (n_1\lambda_{1133}u_{33})^2\Omega_{11}. \quad (\text{A2.2})$$

We can easily calculate the Ω^{-1} tensor in the isotropic medium because

$$\Omega_{ij}^{-1}(\mathbf{n}) = \lambda_{ijkl}n_k n_l = \frac{\mu}{1 - 2\sigma}n_i n_j + \mu\delta_{ij} \quad (\text{A2.3})$$

and then the inverse tensor

$$\Omega_{ij}(\mathbf{n}) = \frac{\delta_{ij}}{\mu} - \frac{1}{2\mu(1 - \sigma)}n_i n_j. \quad (\text{A2.4})$$

After substitution in the expression for $A(\beta)$

$$B(n_1, n_3) = B(\beta) \\ A(\beta) = B(\beta' = 90^\circ) - B(\beta) = \frac{2\mu}{1 - \sigma}(1 - \sin^4 \beta)u_{33}^2. \quad (\text{A2.5})$$

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