Flat elasticity theory application for the description of stressed state and fracture of solids under phase transitions

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The stress function is proved to be biharmonic for an elastically isotropic crystal undergoing phase transition which follows spontaneous dilatation. For an elastically anisotropic crystal which is neither improper nor proper ferroelastic, as well as for the improper ferroelastic, the stress function is proved to fulfil the Lehnitsky equation. The flat elasticity theory methods are extended to the case of crystals undergoing phase transitions. The stressed state, arising due to the phase transition in a crystal with a crack or with a rigid inclusion, is described. The spontaneous fracture conditions of crystals under phase transitions are obtained.

1. Introduction

It is well-known that the phase transitions (PTs), (especially the first-order PTs) in crystals or ceramics often result in their fracture. The main fracture origin is the spontaneous deformation, which can give rise to stress concentration at the inhomogeneities.

The technical application of crystals, ceramics and composities undergoing PTs gives rise to the problem of describing the mechanics of such materials, primarily in relation to their stressed–strained state. In order to solve this problem it is necessary to extend the methods of elastic theory to the case of an elastic body exhibiting non-linear properties arising due to the PT, and to determine the correspondence of the mechanical and thermodynamic properties of the above solids.

In this paper the mathematical apparatus which makes it possible to solve the important class of the above problems (the description of a flat stressed state of solid undergoing PT) is constructed. For an elastically isotropic solid in which the dilatant PT of a second order or of a manifested first order, took place, the stress function is proved to fulfil the linear biharmonic equation in spite of the non-linearity of the state equation. In the elastically anisotropic crystals (which are neither ferroelastics nor improper ferroelastics, as well as for the improper ferroelastics) the Lehnitsky equation is proved to be true for the stress function. The relations of Kolosov–Mus'helishvily potentials [1] (or of Lehnitsky potentials [2, 3]) with the stress tensor and displacement vector are obtained. This generalization makes it possible to use the effective methods of two-dimensional mechanics (as the conformal transformation method) for the case of solids undergoing PTs. Two types of problem, homophase and inhomophase, should be considered in these solids. In the homophase problem the elaborated generalization makes it possible to obtain the solution directly in analogy to the problem in a solid without PT, the solution being exact if it was exact in a solid without PT.

As an example of the application of this method, the problems of a crack and a rigid inclusion in solids undergoing PTs are considered. The exact solutions are obtained for the case of an elastically isotropic solid in which a dilatant PT had taken place, and for an improper ferroelastic with cubic elastic anisotropy and both dilatant and shear spontaneous deformation. The spontaneous fracture conditions of crystals undergoing PTs are obtained.

The spontaneous fracture conditions are estimated using the examples of ferroelectrics $BaTiO_3$, $PbTiO_3$, $KTa_{1-x}Nb_xO_3$, and the improper ferroelastic ZrO_2. The estimations showed that in these crystals the defects of the length $L \simeq 1$ μm cause crystal fracture even at the point of PT (which in these crystals are PTs of the first order). The estimation for high-temperature superconductors showed that defects of length $L \simeq 100$ μm cause fracture of these materials at temperature $T \simeq T_c - 10$ K, where T_c is the temperature of the transition into superconducting phase.

2. Flat elasticity theory in an elastically isotropic solid undergoing phase transition

Consider the free energy describing a PT

$$F = \int_V \left\{ f_{el}(u_{ik}) + \frac{1}{2} g(\nabla\eta)^2 + f(\eta) + f_{st}(\eta, u_{ik}) \right\} dV - \int_S P_i u_i \, dS \qquad (1)$$

where u_{ik} is the strain tensor, η the order parameter (OP) describing the PT [4], V the solid volume, S that part of the surface to which the forth P_i is applied, u_i the displacement vector.

Consider first the simplest case of the second-order PT which is described by one-component OP in the elastically isotropic solid. In this case

$$f_{el}(u_{ik}) = \frac{\lambda}{2}u_{ii}^2 + \mu u_{ik}^2 \quad (2)$$

$$f(\eta) = \frac{1}{2}\alpha\eta^2 + \frac{1}{4}\beta\eta^4 \quad (3)$$

$$f_{st}(\eta, u_{ik}) = A\eta^2 u_{ii} \quad (4)$$

where λ and μ are elastic constants, g, α, β are the phenomenological constants, ($g > 0$, $\alpha = a(T - T_c)$, $a > 0$), T is the temperature, and T_c the Curie temperature. In the case of PTs generated by defect dissolution, $\alpha = a(c - c_c)$, where c is the defect concentration, c_c its value at the PT point. In the case of a second-order PT, $\beta > 0$.A is the striction factor.

If the inhomogeneity scale (the size of the crack or inclusion) $L \gg r_c$, where $r_c \sim (g/\alpha)^{1/2}$ (the OP correlation length) the gradient term in Equation 1 can be neglected. (In the homophase problems, the gradient term, if neglected, results in mistakes in a small vicinity $\sim r_c$ near the stress concentrator. For most crystals undergoing structural PTs, r_c is small; for example, for ferroelectrics its value runs from several to several tens of lattice parameters [5]. Taking the gradient term into account becomes important in heterophase small nuclei problems [6–8]. In the case of a nucleus of size $L \gg r_c$, the gradient term can also be neglected.)

Minimization of Equations 1–4 with respect to OP and u_i gives

$$\begin{cases} \alpha\eta + \beta\eta^3 + 2A\eta u_{ii} = 0 \\ \dfrac{\partial\sigma_{ik}}{\partial x_k} = 0 \\ \sigma_{ik}n_k|_S = P_i(S) \end{cases} \quad (5)$$

where n_k is the surface normal unit. The stress tensor has the form

$$\sigma_{ik} = \lambda u_{jj}\delta_{ik} + 2\mu u_{ik} + A\eta^2\delta_{ik} \quad (6)$$

The potential Equation 1–4 and the equations of state, Equations 5 and 6 describing the second-order PT from the high-symmetry phase, $\eta = 0$, into the low-symmetry phase $\eta = \eta(x, y) \neq 0$.

It is well-known [1, 9], that the equations of the mechanical equilibria (Equation 5) are in a two-dimensional case identically fulfilled if the stress tensor components are expressed with the help of the stress function $U(x, y)$

$$\frac{\partial^2 U}{\partial x^2} = \sigma_{yy}; \quad \frac{\partial^2 U}{\partial y^2} = \sigma_{xx}; \quad \frac{\partial^2 U}{\partial x \partial y} = -\sigma_{xy} \quad (7)$$

under $\eta = 0$ (in other words in the usual elastically isotropic solid) the equation $\Delta\Delta U(x, y) = 0$ is true for the stress function [1]. Here $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$.

It is proved in Appendix 1 that the equation $\Delta\Delta U(x, y) = 0$, is true in the low-symmetry phase, also in the case of a stationary temperature distribution $\Delta T(x, y) = 0$ (or stationary distribution of a concentration $\Delta c(x, y) = 0$), which results in $\Delta\alpha(x, y) = 0$. This result makes it possible to describe a flat stressed state of a low-symmetry phase with the help of the apparatus of complex potentials of Kolosov and Mus'helishvily $\phi(z)$ and $\psi(z)$, where $z = x + iy$ is the complex coordinate. The stress tensor components are expressed with the help of $\phi(z)$ and $\psi(z)$ as

$$\begin{cases} \sigma_{xx} + \sigma_{yy} = 4\mathrm{Re}\phi'(z) \\ \sigma_{yy} - \sigma_{xx} + 2i\sigma_{xy} = 2[\bar{z}\phi''(z) + \psi'(z)] \\ \sigma_{zz} = \tilde{\nu}(\sigma_{xx} + \sigma_{yy}) \\ i\int_{S(t_0)}^{S(t)} (X_n + iY_n)\, ds = \phi(t) + t\overline{\phi'(t)} + \overline{\psi(t)} \end{cases} \quad (8)$$

where the primes indicate the derivative with respect to z, the bars indicate the complex conjugation, $s(t)$ the contour arc, X_n, Y_n the external force components, and $\tilde{\nu} = \tilde{\lambda}/2(\tilde{\lambda} + \mu)$ the Poisson's ratio in the phase $\eta \neq 0$.

For the displacement vector $u_x = u$, $u_y = v$ it is obtained from

$$2\mu(u + iv) = \mathscr{H}\phi(z) - z\overline{\phi'(z)} - \overline{\psi(z)} + Cz \quad (9)$$

where $\mathscr{H} = (\tilde{\lambda} + 3\mu)/(\tilde{\lambda} + \mu)$. Equation 9 corresponds to the case of when temperature (or concentration) together with α is independent of the coordinates.

Consider first the case of a flat spontaneous dilatation, supposing that the spontaneous deformation $u_{ik}^{(0)}$ under the PT is $u_{xx}^{(0)} = u_{yy}^{(0)} \neq 0$; $u_{zz}^{(0)} = u_{xy}^{(0)} = u_{xz}^{(0)} = u_{yz}^{(0)} = 0$. $f_{St} = A\eta^2(u_{xx} + u_{yy})$. The flat spontaneous dilatation is a rather exotic case. However, it is shown below that the other realistic cases of spontaneous dilatation can be reduced to this simple case by means of re-designation of variables. In the case of flat dilatation

$$C = -\frac{\mu A}{\tilde{\lambda} + \mu}\tilde{\eta}^2; \quad \tilde{\eta}^2 = -\frac{\alpha}{\beta}; \quad \tilde{\lambda} = \lambda - \frac{2A^2}{\beta} \quad (10)$$

In the case of the first-order PT, which is close to the second order, $\beta < 0$ and $f(\eta)$ should be taken in the form

$$f(\eta) = \frac{1}{2}\alpha\eta^2 + \frac{1}{4}\beta\eta^4 + \frac{1}{6}\gamma\eta^6 \quad (11)$$

$\gamma > 0$, $\beta < 0$. PT takes place under $\alpha = \alpha_0 = 3\beta^2/16\gamma$. It is not difficult to see that in the case of a first-order PT in the vicinity of a tricritical point $\alpha = \beta = 0$, the linear η^2 dependence on u_{ii} is not realized, together with the stress function biharmonity.

However, in many experiments, the dependence of OP on temperature can be approximated by

$$\eta^2 = \begin{cases} 0, & \alpha_{ef} > \alpha_0 \\ \eta_0^2 - b(\alpha_{ef} - \alpha_0), & \alpha_{ef} \leq \alpha_0 \end{cases} \quad (12)$$

where $\alpha_{ef} = \alpha + 2Au_{ii}(x, y)$, α_0 its value at a PT point (under $\alpha = \alpha_0$ the phases $\eta = 0$ and $\eta \neq 0$ energies are equal), $b > 0$. At the PT point, the OP has a jump η_0, not far from the OP saturation value. With a subsequent decrease in temperature, a slow OP increase takes place. (For example, the polarization in ferroelectrics KDP, KHP [10], $BaTiO_3$, $PbTiO_3$ [5, 10], SbSJ [11] demonstrates the behaviour of this sort.)

Using Equation 10 one can obtain $\eta_0^2 = 3|\beta|/4\gamma$; $b = 2/|\beta|$; $\alpha_0 = 3\beta^2/16\gamma$, which establishes the correspondence of Equation 12 to the results obtained in the framework of the Landau theory. However Equation 12, being applicable in the region of the phase diagram where the Landau theory is true, can be used in the saturation region where the Landau theory does not take place (though Equation 6 is true).

PTs well-described by Equation 12 are termed "the PTs of a manifested first order". For this case, Equations 8 and 9 can be obtained where

$$\tilde{\lambda} = \lambda - 2A^2 b \quad (13a)$$

$$C = -\frac{\mu A}{\tilde{\lambda} + \mu}\tilde{\eta}^2 \quad (13b)$$

$$\tilde{\eta}^2 = \eta_0^2 - b(\alpha - \alpha_0) \quad (13c)$$

In this paper, $\tilde{\eta}$ is used in both cases of PTs; its value is given by Equation 10 in the second-order case, and by Equation 13 in the case of a PT of a manifested first order.

3. The flat problem in the case of three-dimensional spontaneous dilatation

Free energy always contains the term

$$f_{St} = A\eta^2(u_{xx} + u_{yy} + u_{zz}) \quad (14)$$

which generates the three-dimensional spontaneous dilatation. (Under the PTs with elementary cell multiplication there is no other striction terms except Equation 14, η^2 being replaced by the sum of squares of OP components in the case of a multicomponent OP. The exceptions are the improper ferroelastics, considered further.) It is shown in Appendix 2 that this case is reduced to that considered above with the help of the replacement of C by

$$C_1 = \frac{2(\tilde{\lambda} + \mu)}{3\tilde{\lambda} + 2\mu}C \quad (15)$$

Consider the problem of a flat stressed state of a thin plate undergoing PT with the three-dimensional dilatation (Equation 14). It is shown in Appendix 2 that the results of Equations 8 and 9 can be used in this case again, if $\tilde{\lambda}$ and C are replaced in these equations

$$\lambda_2 = \frac{2\mu\tilde{\lambda}}{\tilde{\lambda} + 2\mu}; \quad C_2 = \frac{2\mu}{\tilde{\lambda} + 2\mu}C \quad (16)$$

In this case all quantities should be considered which have been averaged over the plate width.

Equations 8 and 9 give the flat elasticity theory relations for the case of an elastically isotropic solid and a dilatant PT. However, real crystals often demonstrate strong elastic anisotropy, some of them undergoing shear spontaneous deformation under the PT. Consider this case for the examples of PT with spontaneous dilatation in a cubic crystal, and of PT with both spontaneous shear and dilatation in a cubic improper ferroelastic.

4. Relationships of flat theory of elasticity in anisotropic crystals under phase transitions

Some additional conditions on the elastic constants have to be fulfilled in order for the problem in an anisotropic solid to be flat [3]. They can be fulfilled only occasionally under general crystal orientation; however, there is a set of crystallographic classes in which these conditions are always fulfilled for the case of a basic plane coinciding with the xy plane: $D_2(222)$; $C_{2v}(mm2)$; $D_{2h}(mmm)$; $C_4(4)$; $S_4(\bar{4})$; $C_{4h}(4/m)$; $D_4(422)$; $C_{4v}(4mm)$; $D_{2d}(\bar{4}2m)$; $D_{4h}(4/mmm)$; $C_6(6)$; $C_{3h}(\bar{6})$; $C_{6h}(6/m)$; $D_6(622)$; $C_{6v}(6mm)$; $D_{3h}(6m2)$; $D_{6h}(6/mmm)$; $T(2\ 3)$; $T_h(m3)$; $O(432)$; $T_d(\bar{4}3m)$; $O_h(m3m)$.

Consider a cubic crystal undergoing PT which is described by the n-component OP, $\eta = (\eta_1, \eta_2, \ldots, \eta_n)$

$$f_{el} = \frac{1}{2}c_{11}(u_{xx}^2 + u_{yy}^2 + u_{zz}^2) + c_{12}(u_{xx}u_{yy} + u_{xx}u_{zz} + u_{yy}u_{zz}) + c_{44}(u_{xy}^2 + u_{xz}^2 + u_{yz}^2) \quad (17)$$

$$f(\eta) = \frac{1}{2}\alpha\eta^2 + \frac{1}{4}\beta_1(\eta^2)^2 + \frac{1}{4}\beta_2 J_4(\eta) \quad (18)$$

where $\eta^2 = \sum_{i=1}^{n}\eta_i^2$, $J_4(\eta)$ is the fourth order anisotropic invariant (if it exists). In the case of $BaTiO_3$ or $PbTiO_3$, for example, it has the form $J_4(\eta) = \sum_{i=1}^{3}\eta_i^4$.

Under PTs in crystals which are neither proper nor improper ferroelastics, the striction term gains the form of Equation 14.

Consider the most-often realized one-parameter phases: the phases in which $\eta_1 = \eta \neq 0$; $\eta_2 = \eta_3 = \ldots = \eta_n = 0$, or $\eta_1 = \eta_2 = \eta \neq 0$; $\eta_3 = \eta_4 = \ldots = \eta_n = 0$, etc. The flat elastic problem for this case is reasonably to be considered in a more general statement for the case of a cubic improper ferroelastic with a shear spontaneous deformation (the improper ferroelastics are the crystals undergoing PTs, describing by multicomponent OP, the striction term being composed both of dilatant and undilatant terms. The improper ferroelastics are all crystals which are not proper ferroelectrics and which undergo PTs without elementary cell multiplication (for example, all ferroelectrics [5, 10]) and some crystals undergoing PTs with elementary cell multiplication (some antiferroelectrics [5], ZrO_2 [12], etc.). In one-parameter phases the structure of the striction term is simplified, taking the form of η^2, multiplied by the linear combination of u_{ik}. The main features of the improper ferroelastics can be studied within the example of striction term of Equation 19):

$$f_{St} = A\eta^2(u_{xx} + u_{yy} + u_{zz}) + D\eta^2 u_{xy} \quad (19)$$

where D = zero in a previous case, η is the value of multicomponent OP components which are equal to each other, $f(\eta)$ and $f_{el}(u_{ik})$ are given by Equations 17 and 18. Details of the Lehnitsky relations obtaining for this case are given in Appendix 3. For stresses they have the form

$$\begin{aligned}\sigma_{xx} &= 2\mathrm{Re}[\delta_1^2\phi'(z_1) + \delta_2^2\psi'(z_2)]\\ \sigma_{yy} &= 2\mathrm{Re}[\phi'(z_1) + \psi'(z_2)]\\ \sigma_{xy} &= -2\mathrm{Re}[\delta_1\phi'(z_1) + \delta_2\psi'(z_2)]\\ \int_0^s Y_n\mathrm{d}s + C_1 &= 2\mathrm{Re}[\phi(z_1) + \psi(z_2)] \qquad (20)\\ \int_0^s X_n\mathrm{d}s + C_2 &= 2\mathrm{Re}[\delta_1\phi(z_1) + \delta_2\psi(z_2)]\end{aligned}$$

$C_{1,2}$ are the constants. The expression for the displacement vector takes the form

$$\begin{cases} u = 2\mathrm{Re}[p_1\phi(z_1) + p_2\psi(z_2)] - [G_1x + G_2y]\tilde{\eta}^2\\ v = 2\mathrm{Re}[q_1\phi(z_1) + q_2\psi(z_2)] - [G_1y + G_2x]\tilde{\eta}^2\end{cases} \qquad (21)$$

where

$$p_{1,2} = s_{11}\delta_{1,2}^2 + s_{12} - s_{14}\delta_{1,2};$$

$$q_{1,2} = \frac{s_{11} + s_{12}\delta_{1,2}^2 - s_{14}\delta_{1,2}}{\delta_{1,2}} \qquad (22)$$

$$G_1 = \frac{2c_{44}A}{D_1}; \quad G_2 = \frac{(c_{11} + 2c_{12})D}{D_1} \qquad (23)$$

$D_1 = 2\tilde{c}_{44}(\tilde{c}_{11} + 2\tilde{c}_{12}) + 3c_{14}^2$. $\delta_{1,2}$ are the pair of solutions of a characteristic Equation A19 which are not conjugated. $\mathrm{Im}\delta_1 > \mathrm{Im}\delta_2$. s_{ij} values are given by Equation A14. In the case of a second-order PT, $\tilde{c}_{ij}$ are given by Equation A14 and in the case of the PT of a manifested first order, by Equation A22 (Appendix 3). We should mention that there are unrenormed c_{ij} values in the numerators of the Equation 23 and renormed in D_1.

The equilibria conditions for the phase $\eta \neq 0$ are $\tilde{c}_{11} > 0$, $\tilde{c}_{11}^2 - \tilde{c}_{12}^2 > 0$, $D_1 > 0$ and, in the case of a second-order PT, $\alpha_{ef} = \alpha + 2A(u_{xx} + u_{yy} + u_{zz}) + 2Du_{xy} < 0$ (in the first-order PT case the last inequality is replaced by $\alpha_{ef} < \alpha_0$).

Equations 20–23 make it possible to describe the flat stressed state both in an improper ferroelastic and in a crystal which is neither improper nor proper ferroelastic. In the latter case, $G_2 = 0$. The form of Equations 20 is equal to that in a crystal without any PT [3], or in the high-symmetry phase, and differs from the high-symmetry phase relations by the values of $\delta_{1,2}$. The relations for the displacement vector in the phase $\eta \neq 0$ (Equation 21) differs from that in the phase $\eta = 0$ by the terms $\tilde{\eta}^2$ describing spontaneous dilatation and shear.

Equations 8, 9, 20 and 21 make it possible to reduce the problem of stress-state determination in a transformed solid to the boundary problem for the complex potentials. Consider them within the example of a problem of determination of the stress concentration arising at the tip of the crack or at a thin inclusion due to a PT in a solid.

5. Stress concentration generated due to a phase transition on the crack tip

Consider the low-symmetry phase of a crystal. In the case of a second-order PT it should be supposed $\alpha < 0$, and in the case of a first-order PT, $\alpha < \alpha_0$.

Consider first the problem of a stress applied to the boundary of solid. It is not difficult to see that in the case of the elastically isotropic solid, the expressions for σ_{ik} in the phases $\eta = 0$ and $\eta \neq 0$ do not differ from each other. Thus stress distributions in these phases are equal.

In the elastically anisotropic solid, stress distribution in the phase $\eta \neq 0$ differs from that in the phase $\eta = 0$ due to the $\delta_{1,2}$ dependence on the elastic constant values in these phases (Equation 23). However, the displacement given on the crystal boundary results in additional stress which can be the origin of fracture.

Consider the infinite constrained crystal with the thin brittle crack of length 2L. Consider two cases of constraint: (1) $u_{ij}(\infty) = 0$; (2) $u_{yy}(\infty) = 0$ in the elastically isotropic solid with the flat dilatation. The exact solution of this problem is given in Appendix 4.1. The stress asymptotic near the crack tip $x = L + \rho$; $y = 0$ ($\rho \ll L$) is

$$\sigma_{yy} = \frac{A}{V_{1,2}}\tilde{\eta}^2\left(\frac{2L}{\rho}\right)^{1/2} \qquad (24)$$

where $V_1 = 2$, $V_2 = (\tilde{\lambda} + 2\mu)/\mu$ correspond to the constraints of types 1 and 2. The cracking condition following from Equation 24 has the form

$$\tilde{\eta}^2L^{1/2} = \frac{V_{1,2}K_{IC}}{2A\pi^{1/2}} \qquad (25)$$

In the case of the improper ferroelastic considered here, the constraint $u_{xy}(\infty) = 0$ also generates the stressed state. The exact solution is given in Appendix 4.2. The crack tip stress asymptotic ($x = L + \rho$; $y = 0$; $\rho \ll L$) has the form

$$\sigma_{xy} = D\tilde{\eta}^2\left(\frac{2L}{\rho}\right)^{1/2} \qquad (26)$$

from which it follows that the cracking condition

$$\tilde{\eta}^2L^{1/2} = \frac{K_{IIC}}{2D\pi^{1/2}} \qquad (27)$$

6. Stress concentration on a thin inclusion in the low-symmetry phase

The inclusion which elastic constants differ from that of a crystal, being connected with the crystal by the displacement continuity condition on its boundary, is both the origin and the concentrator of stress.

Consider a thin rigid inclusion of the length $2L$. The boundary conditions are $u(x, 0) = v(x, 0) = 0$, $-L \leq x \leq L$, from which in the elastically isotropic case it follows (Appendix 4.3) that the asymptotics at the inclusion tip ($y = 0$; $x = L + \rho$; $\rho \ll L$) are

$$\begin{aligned}\sigma_{yy} &= \frac{C(\tilde{\mathscr{H}} - 1)}{4\tilde{\mathscr{H}}}\left(\frac{2L}{\rho}\right)^{1/2}\\ \sigma_{xx} &= -\frac{C(\tilde{\mathscr{H}} + 3)}{4\tilde{\mathscr{H}}}\left(\frac{2L}{\rho}\right)^{1/2}\end{aligned} \qquad (28)$$

The sign of the striction constant A shows the orientation of stretching stress along or across the inclusion.

Two values of critical temperature correspond to these two cases. If $A < 0$ the crack arises along the inclusion under $T \leq T_{1cr}$; and if $A > 0$ the crack arises across the inclusion under $T \leq T_{2cr}$. The critical temperature values can be determined from the fracture conditions

$$\begin{cases} \tilde{\eta}_{1cr}^2 L^{1/2} \dfrac{2(\tilde{\lambda} + \mu) K_{IC} \mathscr{H}}{\mu |A| (\mathscr{H} - 1)\pi^{1/2}}, & (A > 0) \\ \tilde{\eta}_{2cr}^2 L^{1/2} = \dfrac{2(\tilde{\lambda} + \mu) K_{IC} \mathscr{H}}{\mu A (\mathscr{H} + 3)\pi^{1/2}}, & (A < 0) \end{cases} \quad (29)$$

The exact solution for the case of the thin rigid inclusion in the improper ferroelastic is given in Appendix 4.4. The stress asymptotics are

$$\begin{cases} \sigma_{xx} = -\left(\dfrac{2L}{\rho}\right)^{1/2} \mathrm{Re}\left[\dfrac{G_1(q_1 - q_2) - G_2(p_1 - p_2)}{p_1 q_2 - p_2 q_1}\right]\tilde{\eta}^2 \\ \sigma_{yy} = -\left(\dfrac{2L}{\rho}\right)^{1/2} \mathrm{Re}\left[\dfrac{G_1(\delta_2^2 q_1 - \delta_1^2 q_2) - G_2(\delta_2^2 p_1 - \delta_1^2 p_2)}{p_1 q_2 - p_2 q_1}\right]\tilde{\eta}^2 \\ \sigma_{xy} = -\left(\dfrac{2L}{\rho}\right)^{1/2} \mathrm{Re}\left[\dfrac{G_1(\delta_1 q_2 - \delta_2 q_1) - G_2(\delta_1 p_2 - \delta_2 p_1)}{p_1 q_2 - p_2 q_1}\right]\tilde{\eta}^2 \end{cases} \quad (30)$$

Equation 30 can be used for calculation for concrete crystals and makes it possible to obtain the cracking conditions, but, in a general case, it has a too complicated form. In the elastically isotropic approximation ($c_{11} - c_{12} = 2c_{44}$), the stresses generated by dilatant and by shear spontaneous deformations are independent. The spontaneous dilatation generates stresses for which the asymptotics are given by Equation 28, though the spontaneous shear generates a shear stress which has asymptotics

$$\sigma_{xy} = -\frac{(\tilde{c}_{11} + \tilde{c}_{12})^2 D}{(\tilde{c}_{11} - \tilde{c}_{12})(\tilde{c}_{12} + 3\tilde{c}_{11})}\tilde{\eta}^2 \left(\frac{2L}{\rho}\right)^{1/2} \quad (31)$$

from which it follows the cracking condition

$$\tilde{\eta}^2 L^{1/2} = \frac{K_{IIC}(\tilde{c}_{11} - \tilde{c}_{12})(\tilde{c}_{12} + 3\tilde{c}_{11})}{2(\tilde{c}_{11} + \tilde{c}_{12})^2 D \pi^{1/2}} \quad (32)$$

The cracking conditions (Equations 25 and 29) are obtained for the flat dilatation case. In the case of a three-dimensional dilatation, the right-hand part of Equations 25 or 29 should be multiplied by $(3\tilde{\lambda} + 2\mu)/\{2(\tilde{\lambda} + \mu)\}$, and in the case of a thin plate, $\tilde{\lambda}$ should be replaced in Equations 25 and 29 by λ_2 (Equation 16) and after that the right-hand part of (Equations 25 and 29) should be multiplied by $(\tilde{\lambda} + 2\mu)/2\mu$.

We should mention that K_{IC} and K_{IIC} used in previous sections are the phase $\eta \neq 0$ fracture toughness values, which is why it is necessary to determine their correspondence to the values of fracture toughness in the phase $\eta = 0$.

7. Fracture toughness in a low-symmetry phase

Consider the fracture toughness influence on the PT within the example of the elastically isotropic crystal described by the potential (Equations 1–4) with the crack opened by the stress $\sigma_{yy}(\infty) = P$.

In the phase $\eta = 0$, the energy fracture criterion can be obtained by variation of the difference of the free energy of the crystal with and without a crack: $\Delta F = -P^2 L^2 \pi(1 - \nu_0^2)/E_0 + 4\sigma L$, where E_0 is the Youngs' modulus, ν_0 Poisson's ratio in the phase $\eta = 0$, σ is the surface energy. Thus the well-known Griffiths criterion follows: $(K_{IC}^{(0)} = \{2\sigma E_0/(1 - \nu_0^2)\}^{1/2}$.

Substituting the Equations A1 and A2 into the Equation 1, one can obtain in the low-symmetry phase

$$f = \frac{\tilde{\lambda}}{2} u_{ii}'^2 + \mu u_{ik}'^2 - \frac{1}{1 - \Xi}\frac{\alpha^2}{4\beta} \quad (33)$$

$$\Xi = \frac{2A^2}{\beta(\lambda + \mu)} \quad (34)$$

where $u_{ik}' = s_{ijkl}\sigma_{kl}$. In the expression for ΔF, the last term in Equation 33 vanishes and the first two terms correspond to the case of the elastically isotropic solid with the renormed value of λ. Thus it follows that the fracture toughness values ratio is

$$\left(\frac{K_{IC}}{K_{IC}^{(0)}}\right)^2 = (1 - \Xi)/[1 - (\Xi/2(1 - \nu_0))] \quad (35)$$

The stability condition of the phase $\eta \neq 0$ results in the inequality $\Xi < 1$. Taking into account $\nu_0 < 0.5$ [9] it is not difficult to find that the denominator of Equation 35 never becomes zero. The ratio in Equation 35 is monotonically decreasing with increasing $\Xi \in [0, 1]$.

8. Discussion

The cracking conditions obtained in the previous sections make it possible to determine the critical value of a crack or of a thin inclusion, L_{cr}. Cracking takes place under $L \geq L_{cr}$. It has a catastrophic character in the case of a constrained crystal and a non-catastrophic character in the case of a thin inclusion. In the case of a second-order PT, it is not difficult to obtain $L_{cr} \sim (T - T_c)^{-2}$, thus there are no dangerous cracks near the second-order PT points.

However, in the case of first-order PTs, cracks of critical size exist even at the PT points.

Estimating for ferroelectrics $BaTiO_3$, $PbTiO_3$, $KTa_{1-x}Nb_xO_3$ $A \simeq 10^9$–10^{10} Pa m C^{-2}; $\eta_0 \simeq 0.1$ C m^{-2} [13]; $K_{IC} \sim 10^5$ Pa m$^{1/2}$ [14], one can obtain for these crystals $L_{cr} \sim 10^{-4}$–10^{-6}m. (The OP for ferroelastics is the polarization vector $\boldsymbol{P}$. For the dielectric ferroelectrics ($PbTiO_3$) the additional relation div$\boldsymbol{P} = 0$ has to be fulfilled, thus the above results can be used only for the phase $\boldsymbol{P} = (0, O, P_z(x, y))$. For the case of the ferroelectric semiconductor ($BaTiO_3$ at the temperature of cubic to tetragonal PT) the polarization is screened, the relation div$\boldsymbol{P} = 0$ disappears and all the above results can be used in all phases, for which point symmetries are listed in Section 3.)

For ZrO_2, estimating $u_{ii}^{(0)} \sim 0.1$ [15]; $\tilde{\lambda} + \mu \simeq 2\times 10^{11}$ Pa [16], one can obtain $A\eta_0^2 \simeq 2\times 10^{10}$ Pa. Using the value $K_{IC} \simeq 10\,\mathrm{MPa\,m^{1/2}}$ [17], one can obtain for ZrO_2, $L_{cr} \simeq 10^{-6}$ m. This estimation is true for a shear suppressment of ZrO_2 as well, because the spontaneous shear under the tetragonal to monoclinic PT in ZrO_2 is of the same order as that of spontaneous dilatation [18].

The above estimations are also true for thin inclusions.

The estimations show that small macroscopic defects of the size ~ 1 μm can result in crystal fracture even at the point of first-order PT.

Great attention is now focused on materials demonstrating high-temperature superconductivity. Thus it seems to be useful to estimate their spontaneous fracture conditions. In order to make the estimations, experimental data can be used. The molar specific heat jump is $\Delta c_{molar}/T_c \simeq 10\,\mathrm{J\,K^{-1}\,mol^{-1}}$ Cu, for $La_{2-x}Sr_xCuO_4$ and for $YBa_2Cu_3O_7$ [19]. The dT_c/dp value lies between 10^{-9} and 10^{-8} K Pa^{-1} in different La–Sr–Cu–O, La–Ba–Cu–O and Y–Ba–Cu–O high-T_c superconductors [20]. The Young modulus value, $E \simeq 10^{11}$ Pa [21, 22]. Taking into account the relation

$$\frac{Aa}{\beta} = \frac{2}{3}(3\lambda + 2\mu)\frac{dT_c}{dp}\frac{\Delta c}{T_c} \qquad (36)$$

where Δc is the specific heat of the unit volume: $\Delta c = \Delta c'\rho/m_0$; the density $\rho \sim 10\,\mathrm{g\,cm^{-3}}$; the molar mass of copper $m_0 \sim 100\,\mathrm{g\,mol^{-1}}$, one can obtain $Aa/\beta \simeq 10^6\,\mathrm{J\,K^{-2}\,m^{-3}}$. Taking the value $K_{IC} \sim 10^5$ Pa m$^{1/2}$ [23], one can obtain using Equation 25 the temperature of spontaneous fracture. For defects of length $L \simeq 10^{-4}$ m, $T \sim T_c - 10$ K, and for defects of length $L \simeq 10^{-6}$ m, $T \sim T_c - 100$ K. Thus large defects $L \simeq 10^{-4}$ m can result in spontaneous fracture of high-temperature superconductors.

The fracture toughness is renormed in a low-symmetry phase. In the elastically isotropic case, its value decreases under PT into phase $\eta \neq 0$. However in the anisotropic case, elastic constant renormalization can result in an additional phenomenon: the direction of the maximal stretching or shear stress can deviate from that in the high-symmetry phase.

Appendix 1. The stress function biharmonity, relations of stress and strain and the complex potentials

The mechanical equilibria, Equations 5, are fulfilled identically in the flat case if the stress tensor components are expressed with the help of the stress function Equation 7.

It is well-known that under $\eta = 0$ (in other words, in an ordinary elastically isotropic solid without any PT) the stress function satisfies the biharmonic equation.

In the phase $\eta = \eta(x, y) \neq 0$ the OP values can be expressed (Equation 5) as

$$\eta^2 = -\alpha_{ef}/\beta; \quad \alpha_{ef} = \alpha + 2Au_{ii}(x, y) \qquad (A1)$$

under $\alpha_{ef} < 0$. Consider first a case of a flat spontaneous dilatation $f_{St} = A\eta^2(u_{xx} + u_{yy})$. In this case the subscripts i, j, k take the values 1, 2. the strain tensor can be expressed as

$$u_{ij} = s_{ijkl}\sigma_{kl} + u_{ij}^{(0)} \qquad (A2)$$

where $u_{xx}^{(0)} = u_{yy}^{(0)} = A\alpha/[2\beta(\tilde{\lambda} + \mu)]$; $u_{xy}^{(0)} = u_{zz}^{(0)} = 0$;

$s_{1111} = s_{2222} \equiv s_{11} = (\tilde{\lambda} + 2\mu)/[4\mu(\tilde{\lambda} + \mu)]$;

$s_{1122} \equiv s_{12} = -\tilde{\lambda}/[4\mu(\tilde{\lambda} + \mu)]$; $s_{1212} \equiv s_{44} = (2\mu)^{-1}$.

The value of λ is renormed under the PT: $\tilde{\lambda} = \lambda - 2A^2/\beta$. The strain tensor components satisfy the Sen-Venan relation [1]

$$\frac{\partial^2 u_{xx}}{\partial y^2} + \frac{\partial^2 u_{yy}}{\partial x^2} = 2\frac{\partial^2 u_{xy}}{\partial x \partial y} \qquad (A3)$$

Substituting Equations A2 and 7 into Equation A3, one can obtain the equation for the stress function in the phase $\eta \neq 0$:

$$\Delta\Delta U(x, y) = 0 \qquad (A4)$$

if $\alpha = \alpha(x, y)$ satisfies the harmonic equation $\Delta\alpha(x, y) = 0$. This condition is fulfilled, of course, in the case $\alpha =$ constant; however, $\alpha = a(T - T_c)$ or $\alpha = a(c - c_c)$ and the condition $\Delta\alpha = 0$ is fulfilled in the more general case of stationary distribution of temperature $\Delta T(x, y) = 0$, or of concentration $\Delta c(x, y) = 0$.

The Equation 2 and Equations 5 and 6 do not take into account the thermal expansion which is usually small in comparison with a striction phenomenon. However, thermal expansion can be taken into account by adding the Equation 2 the term which is linear in temperature and in u_{ll} [9]. In this case the stress function satisfies the biharmonic equation if the condition $\Delta T(x, y) = 0$ is fulfilled. The linear swelling of solid under defect dissolution can be taken into account in an analogous way.

Repeating the arguments [1], one can obtain the relations of the stress tensor components and complex potentials $\phi(z)$ and $\psi(z)$, Equation 8 being equal to that in the high-symmetry phase.

In order to obtain the expression for the displacement vector, u_{xx} and u_{yy} (Equation A2) should be integrated over x and y correspondingly; the terms describing the displacement and the rotation of the plane as a whole should be subtracted. After that, only one undetermined constant is left, which is fixed by the condition $\partial u/\partial y + \partial v/\partial x = 2u_{xy}$. In the case $\alpha =$ constant, it results in Equation 9.

Appendix 2. The stress function biharmonity in a flat problem in the case of the three-dimensional spontaneous dilatation

A2.1. A flat problem in the case of the three-dimensional spontaneous dilatation

In the case of the three-dimensional spontaneous dilatation (Equation 14), the stress–strain relations are

$$\begin{cases} (\tilde{\lambda} + 2\mu)u_{xx} + \tilde{\lambda}(u_{yy} + u_{zz}) + A\tilde{\eta}^2 = \sigma_{xx} \\ (\tilde{\lambda} + 2\mu)u_{yy} + \tilde{\lambda}(u_{xx} + u_{zz}) + A\tilde{\eta}^2 = \sigma_{yy} \\ (\tilde{\lambda} + 2\mu)u_{zz} + \tilde{\lambda}(u_{xx} + u_{yy}) + A\tilde{\eta}^2 = \sigma_{zz} \end{cases} \quad \text{(A5)}$$

Divide the strain tensor into two terms: $u_{xx} = u_0 + u'_{xx}$; $u_{yy} = u_0 + u'_{yy}$; $u_{zz} = u_0$; $u_{xy} = u'_{xy}$

$$u_0 = -\frac{A}{3\tilde{\lambda} + 2\mu}\tilde{\eta}^2 \quad \text{(A6)}$$

from which it follows that

$$\sigma_{zz} = \tilde{\lambda}(u'_{xx} + u'_{yy})$$

$$\begin{cases} (\tilde{\lambda} + 2\mu)u'_{xx} + \tilde{\lambda}u'_{yy} + \dfrac{2(\tilde{\lambda} + \mu)}{3\tilde{\lambda} + 2\mu}A\tilde{\eta}^2 = \sigma_{xx} \\ (\tilde{\lambda} + 2\mu)u'_{yy} + \tilde{\lambda}u'_{xx} + \dfrac{2(\tilde{\lambda} + \mu)}{3\tilde{\lambda} + 2\mu}A\tilde{\eta}^2 = \sigma_{yy} \end{cases} \quad \text{(A7)}$$

This results in a biharmonic equation for $U(x, y)$ and in Equations 8 and 9 in which $\tilde{\eta}^2$ should be replaced by

$$\hat{\eta}^2 = \frac{2(\tilde{\lambda} + \mu)}{3\tilde{\lambda} + 2\mu}\tilde{\eta}^2 \quad \text{(A8)}$$

in the expression for C.

A2.2. PT with three-dimensional dilatation in a thin plate

Consider a flat thin plate of a width $2h$, in which the surfaces are free from stress. The equilibria equation results in $\partial\sigma_{zz}(x, y, \pm h)/\partial z = 0$ because $\partial\sigma_{xz}(x, y, \pm h)/\partial z = \partial\sigma_{yz}(x, y, \pm h)/\partial z = \partial\sigma_{zz}(x, y, \pm h)/\partial z = 0$. It follows that σ_{zz} is small inside the plate, so it can be considered to be $\sigma_{zz} \approx 0$. Substituting this equation into Equation A5, we obtain

$$\begin{cases} \dfrac{2\mu\tilde{\lambda}}{\tilde{\lambda} + 2\mu}(u_{zz} + u_{yy}) + 2\mu u_{zz} + \dfrac{2\mu A}{\tilde{\lambda} + 2\mu}\tilde{\eta}^2 = \sigma_{xx} \\ \dfrac{2\mu\tilde{\lambda}}{\tilde{\lambda} + 2\mu}(u_{zz} + u_{yy}) + 2\mu u_{yy} + \dfrac{2\mu A}{\tilde{\lambda} + 2\mu}\tilde{\eta}^2 = \sigma_{yy} \\ 2\mu u_{xy} = \sigma_{xy} \end{cases} \quad \text{(A9)}$$

from which it appears that the problem is reduced to the case considered above, by the replacement of $\tilde{\lambda}$ and $\tilde{\eta}^2$ by

$$\lambda_2 = \frac{2\mu\tilde{\lambda}}{\tilde{\lambda} + 2\mu}; \quad \hat{\eta}^2 = \frac{2\mu\tilde{\lambda}}{\tilde{\lambda} + 2\mu}\tilde{\eta}^2 \quad \text{(A10)}$$

Appendix 3. Flat theory relations for the improper cubic ferroelastic

Minimum conditions for the Equation 1 with the free energy density (Equations 17–19) results in the state equations

$$\begin{cases} \dfrac{\partial\sigma_{ik}}{\partial x_k} = 0 \\ \alpha\eta_i + \beta_1\eta_i\sum_{i=1}^{n}\eta_i^2 + \dfrac{1}{4}\beta_2\dfrac{\partial I_4}{\partial\eta_i} + 2A\eta_i u_{jj} + 2D\eta_i u_{xy} = 0 \end{cases} \quad \text{(A11)}$$

where

$$\begin{cases} \sigma_{xx} = c_{11}u_{xx} + c_{12}(u_{yy} + u_{zz}) + A\eta^2 \\ \sigma_{yy} = c_{11}u_{yy} + c_{12}(u_{xx} + u_{zz}) + A\eta^2 \\ \sigma_{xx} = c_{11}u_{zz} + c_{12}(u_{xx} + u_{yy}) + A\eta^2 \\ \sigma_{xy} = 2c_{44}u_{xy} + D\eta^2 \end{cases} \quad \text{(A12)}$$

Considering a one-parameter phase and denoting by β a factor multiplied by η^3, one can obtain

$$\alpha\eta + \beta\eta^3 + 2A\eta u_{jj} + 2D\eta u_{xy} = 0 \quad \text{(A13)}$$

The strain tensor should be divided into two parts: $u_{ij} = u_{ij}^{(0)} + u'_{ij}$ and Equation A2 should be obtained in which the elastic compliance factors and $u_{ij}^{(0)}$ for the second-order PT case are

$$\begin{cases} s_{1111} = s_{2222} \equiv s_{11} = \dfrac{2\tilde{c}_{11}\tilde{c}_{44} - c_{14}^2}{D_2}; \quad s_{1122} \equiv s_{12} = -\dfrac{2\tilde{c}_{12}\tilde{c}_{44} - c_{14}^2}{D_2} \\ s_{1112} \equiv s_{14} = -\dfrac{c_{14}(\tilde{c}_{11} - \tilde{c}_{12})}{D_2}; \quad s_{1212} \equiv s_{44} = \dfrac{\tilde{c}_{11}^2 - \tilde{c}_{12}^2}{D_2} \\ D_2 = 2\tilde{c}_{44}(\tilde{c}_{11}^2 - \tilde{c}_{12}^2) - 2c_{14}^2(\tilde{c}_{11} - \tilde{c}_{12}) > 0 \\ \tilde{c}_{11} = c_{11} - \dfrac{2A^2}{\beta}; \quad \tilde{c}_{12} = c_{12} - \dfrac{2A^2}{\beta}; \quad \tilde{c}_{44} = c_{44} - \dfrac{D^2}{\beta} \\ c_{14} = -\dfrac{2AD}{\beta}; \quad u_{xx}^{(0)} = u_{yy}^{(0)} = u_{zz}^{(0)} = -\dfrac{2c_{44}A}{D_1}\tilde{\eta}^2 \\ u_{xy}^{(0)} = -\dfrac{(c_{11} + 2c_{12})D}{D_1}\tilde{\eta}^2; \quad D_1 = 2\tilde{c}_{44}(\tilde{c}_{11} + 2\tilde{c}_{12}) + 3c_{14}^2 > 0 \end{cases} \quad \text{(A14)}$$

Note that c_{ij} values in the numerator of the expressions for $u_{ij}^{(0)}$ (Equation A14) are unrenormed.

Using Equations A2, A3 and A14 one can obtain the Lehnitsky equation for the stress function

$$s_{11}(U_{xxxx} + U_{yyyy}) + 2(s_{12} + s_{44})U_{xxyy} - 3s_{14}(U_{xyyy} + U_{xxxy}) = 0 \quad \text{(A15)}$$

where $U_{xxxx} = \partial^4 U/\partial x^4$; $U_{xxyy} = \partial^4 U/\partial x^2\partial y^2$, etc, if

$\alpha = \alpha(x, y)$ satisfies the equation

$$\Delta\alpha = \frac{c_{11} + 2c_{12}}{c_{44}}\frac{D}{A}\frac{\partial^2\alpha}{\partial x\partial y} \qquad (A16)$$

from which it follows that Equation A15 holds in the case of stationary temperature distribution $\Delta T(x, y) = 0$, if $D = 0$. If $D \neq 0$, Equation A15 holds for the case α = constant.

The solution to Equation A15 should be tried in the form

$$U = F_1(z_1) + F_2(z_2) + \overline{F_1(z_1)} + \overline{F_2(z_2)} \qquad (A17)$$

where

$$z_{1,2} = x + \delta_{1,2}y \qquad (A18)$$

where $\delta_{1,2}$ are the pair of unconjugated solutions of the Equation 18

$$s_{11}\delta^4 - 3s_{14}\delta^3 + 2(s_{12} + s_{44})\delta^2 - 3s_{14}\delta + s_{11} = 0 \qquad (A18)$$

$\mathrm{Im}\delta_1 > \mathrm{Im}\delta_2$. Note that the solutions of Equation A18 are always complex, and even in a cubic phase they can consist of both real and imaginary parts. The existence of $c_{14} \neq 0$ ($s_{14} \neq 0$) in the phase $\eta \neq 0$ is the result of symmetry breaking under the PT. In the case of ferroelastics $BaTiO_3$, $PbTiO_3$ and $KTa_{1-x}Nb_xO_3$ the striction constant can be estimated as $A/E \simeq D/E \simeq 10^{-1}$–$10^{-2}$ m^{4}C^{-2} [13], from which it follows that $s_{14} \simeq A^2/(E^2|\beta|) \simeq 10^{-10}$–$10^{-12}$ Pa^{-1}, although in a cubic phase $s_{ij} \sim 10^{-11}$ Pa^{-1}. Thus s_{14} is not obligatory, and can be neglected in comparison with the other s_{ij} values. If it can be neglected

$$\begin{cases} \delta^2 = -k \pm (k^2 - 1)^{1/2} \\ k = -\dfrac{\tilde{c}_{12}}{\tilde{c}_{11}} + \dfrac{\tilde{c}_{11}^2 - \tilde{c}_{12}^2}{2\tilde{c}_{11}\tilde{c}_{44}} \end{cases} \qquad (A20)$$

Considering the initial phase to be elastically isotropic ($2c_{44} = c_{11} - c_{12}$), one can obtain $k = 1 + \varepsilon(\tilde{c}_{11} + \tilde{c}_{12})/[\tilde{c}_{11}(1 - \varepsilon)]$, where $\varepsilon = D^2/(\beta c_{44})$, and thus the two pairs of imaginary solutions follow. Under $\varepsilon \ll 1$

$$\delta \cong \pm i\{1 \pm [\varepsilon(\tilde{c}_{11} + \tilde{c}_{12})/2\tilde{c}_{11}]^{1/2}\} \qquad (A21)$$

Denoting $dF_1/dz_1 = \phi(z_1)$; $dF_2/dz_2 = \psi(z_2)$ and using Equations A17 and 7, one can obtain the Equations 20. Equations 21 for the displacement vector components can be obtained by integration of Equation A2, using Equation A14 and giving up the terms corresponding to the displacement and rotation of the plane as a whole.

In the case of a PT of a manifested first order, one should use

$$\begin{bmatrix} \tilde{c}_{11} = c_{11} - 2A^2b; & \tilde{c}_{12} = c_{12} - 2A^2b; \\ c_{44} = c_{44} - D^2b; & c_{14} = -2ADb \end{bmatrix} \qquad (A22)$$

and all the above results again hold.

After the problem of determination of stress components σ_{xx}, σ_{yy} and σ_{xy} is solved, σ_{zz} can be obtained with the help of the Equation

$$\sigma_{zz} = [\tilde{c}_{12}(s_{11} + s_{12}) + c_{14}s_{14}] \times (\sigma_{xx} + \sigma_{yy}) + (2\tilde{c}_{12}s_{14} + c_{14}s_{44})\sigma_{xy} \qquad (A23)$$

Appendix 4. Cracks and thin inclusions in a low-symmetry phase: exact solutions

A4.1. Symmetrical flat brittle crack

Consider a flat brittle crack of a length $2L$ situated along Ox symmetrically with respect to the coordinates origin in an infinite elastically isotropic solid under the PT. The state Equations for this case are given by Equations 5 and 6, and the relations of stress and displacement and Kolosov–Mus'helishvily potentials by Equations 9 and 10.

Potentials $\phi(z)$ and $\psi(z)$ have the asymptotics $\phi'(z) \to \Gamma$; $\psi'(z) \to \Gamma'$ under $|z| \to \infty$, Γ being the real and Γ', in the general case, the complex constants [1]. Γ and Γ' values are determined by the conditions in infinity.

If the crystal is constrained, the PT results in an increase of stress which is able to open or close the crack. Consider the cases of constraints (1) $u_{ij}(\infty) = 0$ and (2) $u_{yy}(\infty) = 0$. Using Equations 5, 6 and 9, one can obtain in the first case $\sigma_{xx}(\infty) = \sigma_{yy}(\infty) = A\tilde{\eta}^2$, from which it follows that:

$$\Gamma_1 = A\tilde{\eta}^2/2; \quad \Gamma_1' = 0 \qquad (A24)$$

and in the second case

$$2\Gamma_2 = \Gamma_2' = \frac{\mu A}{\tilde{\lambda} + 2\mu}\tilde{\eta}^2 \qquad (A25)$$

Note that $\tilde{\lambda} > 0$ is the equilibrium condition for the phase $\eta \neq 0$, thus the signs of Γ and Γ' are determined only by the sign of A.

Let the crack be opened due to the normal forces $\sigma_{yy}^+(t) = \sigma_{yy}^-(t) = -p(t)$, $-L \leq t \leq L$, where the superscript + and − are used to denote the stress values on the crack sides.

Thus the problem is reduced to the well-known problem of a flat theory of elasticity [1], which in case (1) has the solution

$$\begin{cases} \phi'(z) = \dfrac{1}{2\pi(z^2 - L^2)^{1/2}}\left[\displaystyle\int_{-L}^{L}\frac{(L^2 - t^2)^{1/2}p(t)\mathrm{d}t}{z - t} + \pi A\tilde{\eta}^2\right] \\ \Omega(z) = \phi'(z) \end{cases} \qquad (A26)$$

where $\Omega(z) = \bar{\phi}'(z) + \bar{z}\bar{\phi}''(z) + \bar{\psi}'(z); \bar{f}(z) \equiv \overline{f(\bar{z})}$
In case (2)

$$\begin{cases} \phi'(z) + \Omega(z) = \dfrac{1}{\pi(z^2 - L^2)^{1/2}} \left[\displaystyle\int_{-L}^{L} \frac{(L^2 - t^2)^{1/2} p(t)\, dt}{z - t} - \frac{\pi\mu A[2z + (z^2 - L^2)^{1/2}]}{\tilde{\lambda} + 2\mu} \tilde{\eta}^2 \right] \\ \phi'(z) - \Omega(z) = \dfrac{\mu A}{\tilde{\lambda} + 2\mu} \tilde{\eta}^2 \end{cases} \quad \text{(A27)}$$

The results of Equations A26 and A27 are exact. They make it possible to obtain the OP and stress distribution in a solid. The asymptotic of stress under $p = 0$ in the crack-tip vicinity is given by Equation 24.

A4.2. Improper cubic ferroelastic

In the case of an improper cubic ferroelastic, consider the suppressing of $u_{xy}(\infty) = 0$, from which it follows that $\sigma_{xy}(\infty) = -D\tilde{\eta}^2$; $\sigma_{xx}(\infty) = \sigma_{yy}(\infty) = 0$. The solution for the Lehnitsky potentials should be tried in the form

$$\begin{cases} \phi(z_1) = Mz_1 + \phi_0(z_1) \\ \psi(z_2) = Bz_2 + \psi_0(z_2) \end{cases} \quad \text{(A28)}$$

where M is real and $B = B' + iB''$. Using the conditions of infinity one can obtain

$$\begin{cases} B'' = \dfrac{D\tilde{\eta}^2}{2} \left[\dfrac{\delta_2'^2 - \delta_2''^2 - \delta_1'^2 + \delta_1''^2}{\delta_2'[\delta_2''^2 - \delta_1''^2 - (\delta_2' - \delta_1')^2]} \right] \\ B' = -M = \dfrac{D\tilde{\eta}^2}{2} \left[\dfrac{2\delta_2'}{\delta_2''^2 - \delta_1''^2 - (\delta_2' - \delta_1')^2} \right] \end{cases} \quad \text{(A29)}$$

where $\delta_{1,2}' = \text{Re}\delta_{1,2}$; $\delta_{1,2}'' = \text{Im}\delta_{1,2}$.

For the crack which is not loaded, $X_n = Y_n = 0$ and the last two of Equations 20 give the boundary conditions for the potentials $\phi_0(z_1)$ and $\psi_0(z_2)$. Consider first the elliptical hole which has the boundary

$$x = \frac{L}{2}(\sigma + \bar{\sigma}); \quad y = \frac{il}{2}(\sigma - \bar{\sigma}) \quad \text{(A30)}$$

where $\sigma = \exp(i\theta)$. After the conformal transformation

$$z_{1,2} = \frac{L + i\delta_{1,2}l}{2}\xi + \frac{L - i\delta_{1,2}l}{2}\frac{1}{\xi} \quad \text{(A31)}$$

(of two different ellipses in complex planes z_1 and z_2 into the unit circle in the complex plain ξ, which is the same for both ellipses) the boundary conditions take the form

$$\begin{cases} \text{Re}[\phi_0(\sigma) + \psi_0(\sigma)] = -\dfrac{D\tilde{\eta}^2}{2}\dfrac{il}{2}(\sigma - \bar{\sigma}) \\ \text{Re}[\delta_1\phi_0(\sigma) + \delta_2\psi_0(\sigma)] = -\dfrac{D\tilde{\eta}^2}{2}\dfrac{L}{2}(\sigma + \bar{\sigma}) \end{cases} \quad \text{(A32)}$$

Integrating Equation A32 with the kern $(\sigma + \xi)\{2\pi i(\sigma - \xi)\sigma^2\}^{-1}$ over the contour of the unit circle and returning to the planes z_1 and z_2, one can obtain the exact solution of the boundary problem (Equation A32)

$$\begin{cases} \phi_0(z_1) = D\tilde{\eta}^2 \dfrac{(L + il\delta_1)(L + il\delta_2)}{\delta_1 - \delta_2} \dfrac{1}{z_1 + [z_1^2 - (L^2 + \delta_1^2 l^2)]^{1/2}} \\ \psi_0(z_2) = -D\tilde{\eta}^2 \dfrac{(L + il\delta_1)(L + il\delta_2)}{\delta_1 - \delta_2} \dfrac{1}{z_2 + [z_2^2 - (L^2 + \delta_2^2 l^2)]^{1/2}} \end{cases} \quad \text{(A33)}$$

The crack case corresponds to the limit $l \to 0$

$$\begin{cases} \phi_0(z_1) = \dfrac{D\tilde{\eta}^2 L^2}{\delta_1 - \delta_2} \dfrac{1}{z_1 + (z_1^2 - L^2)^{1/2}} \\ \psi_0(z_2) = -\dfrac{D\tilde{\eta}^2 L^2}{\delta_1 - \delta_2} \dfrac{1}{z_2 + (z_2^2 - L^2)^{1/2}} \end{cases} \quad \text{(A34)}$$

from which the stress asymptotics (Equation 26) follows

A4.3. Rigid elliptical inclusion in elastically isotropic solid

Consider a rigid elliptical inclusion in the case of the elastically isotropic solid under the PT with a flat dilatation. The condition $u = v = 0$ on the inclusion boundary (Equation A30) after the transformation

$$z = \omega(\xi) = \frac{L + l}{2}\xi + \frac{L - l}{2}\frac{1}{\xi} \quad \text{(A35)}$$

of the ellipse into the unit circle, gives the boundary condition

$$\mathscr{K}\phi(\sigma) - \frac{\omega(\sigma)}{\overline{\omega'(\sigma)}}\bar{\phi}'(\sigma) - \bar{\Psi}(\sigma) = -C\frac{L + l}{2}\left(\sigma + \frac{L - l}{L + l}\bar{\sigma}\right) \quad \text{(A36)}$$

Integration over the contour of a unit circle with the kern $[2\pi i(\sigma - \xi)]^{-1}$, $(|\xi| > 1)$ gives

$$\begin{cases} \phi(\xi) = -\dfrac{C(L-l)}{2\xi}; \\ \psi(\xi) = -\dfrac{C(L+l)}{2\xi}\left[1 + \dfrac{L - 1 + \xi^2(L+l)}{L - l - \xi^2(L+l)}\dfrac{1}{\bar{\mathscr{H}}}\right] \end{cases} \quad \text{(A37)}$$

Equation A37 is the exact solution of the boundary problem (Equation A36). The case of a thin inclusion-corresponds to $l = 0$. Returning to the plane z, one can obtain the asymptotics (Equation 28).

A4.4. Rigid elliptical inclusion in improper ferroelastic

In the case of a rigid elliptical inclusion in an improper ferroelastic, the boundary condition $u = v = 0$ results in the boundary equations

$$\begin{cases} 2\mathrm{Re}[p_1\phi(\sigma) + p_2\psi(\sigma)] \\ = \left\{\dfrac{G_1L + ilG_2}{2}\sigma + \dfrac{G_1L - ilG_2}{2}\bar{\sigma}\right\}\tilde{\eta}^2 \\ 2\mathrm{Re}[q_1\phi(\sigma) + q_2\psi(\sigma)] \\ = \left\{\dfrac{G_2L + ilG_1}{2}\sigma + \dfrac{G_2L - ilG_1}{2}\bar{\sigma}\right\}\tilde{\eta}^2 \end{cases} \quad \text{(A38)}$$

from which it follows that:

$$\begin{cases} \phi(z_1) = -\dfrac{(L + i\delta_1 l)[q_2(G_1L - ilG_2) - p_2(LG_2 - ilG_1)]}{p_1q_2 - p_2q_1}\dfrac{1}{z_1 + [z_1^2 - (L^2 + \delta_1^2l^2)]^{1/2}} \\ \psi(z_2) = -\dfrac{(L + i\delta_2 l)[p_1(G_2L - ilG_1) - q_1(LG_1 - ilG_2)]}{p_1q_2 - p_2q_1}\dfrac{1}{z_2 + [z_2^2 - (L^2 + \delta_2^2l^2)]^{1/2}} \end{cases} \quad \text{(A39)}$$

Turning to the case of a thin inclusion $l = 0$, one can obtain the asymptotics Equation 30. Considering s_{14} and ε to be small in an elastically isotropic crystal, $c_{11} - c_{12} = 2c_{44}$, one can obtain

$$p_1q_2 - p_2q_1 = 2i\left[\frac{\varepsilon(\tilde{c}_{11} + \tilde{c}_{12})}{2\tilde{c}_{11}}\right]^{1/2} \times \frac{\tilde{c}_{12} + 3\tilde{c}_{11}}{(\tilde{c}_{11} + \tilde{c}_{12})(\tilde{c}_{11}^2 - \tilde{c}_{12}^2)} \quad \text{(A40)}$$

$$\delta_1p_2 - \delta_2p_1 = 2i\left[\frac{\varepsilon(\tilde{c}_{11} + \tilde{c}_{12}}{2\tilde{c}_{11}}\right]^{1/2}\frac{1}{\tilde{c}_{11} - \tilde{c}_{12}} \quad \text{(A41)}$$

from which follows the asymptotics Equation 31.

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