Modeling an interaction between a phase transforming inclusion and a crack

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Abstract. Materials may contain inclusions that can endure stress-induced phase transformations. Phase transformations change elasticity modules of a material and produce a transformation strain. As a result, local stresses change. This in turn can initiate or block fracture processes. This work presents the investigations of the interaction between the inclusion enduring phase transformations and a crack. We study the possibility of phase transitions due to the stresses induced by a crack and the influence of the phase transformation on the crack trajectory. The possibility of phase transition in the inclusion is determined by the principle of the energy preference. The study of a crack trajectory is based on the calculation of the stress intensity factors. We develop the finite element method algorithm for the determination of the phase state of the inclusion in arbitrary stress fields. Then we show that the crack growth can initiate phase transitions in the inclusion. We also show that, in dependence of material parameters, the inclusion attracts or repels the crack if the phase transformation takes place. The competition between the external stress field and stresses induced by the phase transformations is demonstrated. Increasing external stress may suppress or intensify the effect of phase transformations, in dependence of material parameters.

Introduction

Materials may contain inclusions which can suffer stress induced phase (structural) transformations under the process of the deformation of a body. We have formulated the problems of phase transformations in the phase-transforming inclusion earlier [1]. The domains of one phase states of the inclusion were constructed analytically in external strain space for the case of the inclusion under uniform external strain field. The possibility of two-phase states of the inclusion was also studied.

The present part of the report is devoted to the studies of the interaction between a phase transforming inclusion and a crack. We developed a numerical procedure for the determination of the current phase state of the inclusion under arbitrary (uniform and non-uniform) external strains (basing on FEM). The procedure was verified by the comparison with the previous analytical results obtained for the case of uniform external fields. Then we studied phase transformations of the inclusion in the stresses induced by the crack at various positions of the straight-line crack and the inclusion. We demonstrated that the crack indeed can produce phase transformations.

Then we studied how the phase transformation in the inclusion affects the trajectory of the crack. We showed that, in dependence of material parameters, the phase transformation leads to the deviation of the crack to the inclusion or from the inclusion. We mentioned that the effects take place when the distance between the tip of the crack and the center of the inclusion is comparable with the diameter of the inclusion (at reasonable choice of the material parameters). This means impossibility of using asymptotic methods and gives additional reasons to develop numerical procedures. We also demonstrated the competition between external field and stresses induced by the phase transformations. Increasing external stress may suppress or intensify the action of the phase transformation, in dependence of material parameters.

Phase state of the inclusion in dependence of external strains and the relative position of the inclusion and the crack. Statement of the problem.

We consider a linear elastic body (the matrix) containing an inclusion which can suffer a phase transitions under an external strain field. Since a material of the inclusion allows phase transformations, its free energy density is to be nonconvex in some means. In a case of small strains it is modeled by piece-wise quadratic dependencies of the strain tensor ε. For the simplicity sake we consider the two-branches dependence [2-6]

$$f(\boldsymbol{\varepsilon},\theta) = \min_{-,+}\{f_-(\boldsymbol{\varepsilon},\theta), f_+(\boldsymbol{\varepsilon},\theta)\} \tag{1}$$

$$f_\pm(\boldsymbol{\varepsilon},\theta) = f_\pm^0(\theta) + \frac{1}{2}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_\pm^p)\cdot\cdot\mathbf{C}_\pm\cdot\cdot(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}_\pm^p),$$

Here plus and minus denote different phase states of the material inside the inclusion, $C_\pm$ are the elasticity tensors of the phases plus and minus, $f_\pm^0$ и $\varepsilon_\pm^p$ are the free energy densities and strain tensors in unstressed phases plus and minus. Further we take $\varepsilon_-^p = 0$, then $\varepsilon_+^p = \varepsilon^p$ is the transformation strain tensor. If $C_\pm$ and $\varepsilon_\pm^p$ does not depend on the temperature θ, and thermoelastic effects are not taken into account, then the parameter $\gamma(\theta) = f_+^0(\theta) - f_-^0(\theta)$ acts as the temperature. One-dimensional analogy of the strain energy density is represented in Fig. 1.

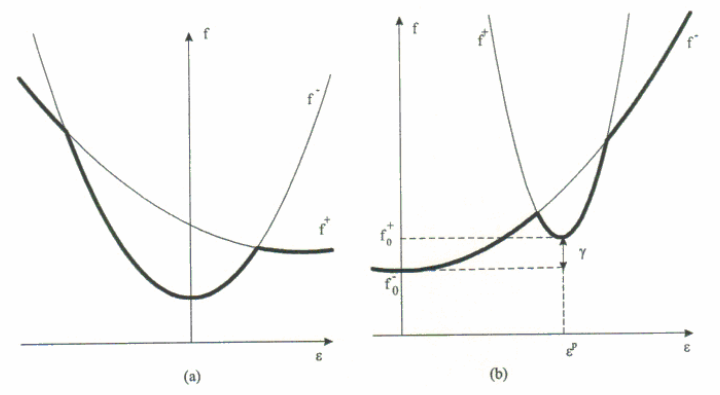

Fig.1: Free energy density at various material parameters

The constitutive equations of the materials of the surrounding matrix and the inclusion in different phase states are given by the relationships

$$\boldsymbol{\sigma}_0 = \mathbf{C}_0\cdot\cdot\boldsymbol{\varepsilon}, \quad \boldsymbol{\sigma}_- = \mathbf{C}_-\cdot\cdot\boldsymbol{\varepsilon}, \quad \boldsymbol{\sigma}_+ = \mathbf{C}_+\cdot\cdot(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^p), \tag{2}$$

where C^0 is the elasticity tensor of the matrix.

In the present consideration we suppose that the inclusion can be in one of two possible phase states. The choice of the phase state provides the minimum of the potential energy of the body.

Let Π_- and Π_+ be the potential energies of the body containing the inclusion in the phase state minus and plus, respectively, and Π_0 be the potential energy of the body without the inclusion at the same boundary conditions. Then

$$F \equiv \Pi_+ - \Pi_- = (\Pi_+ - \Pi_0) - (\Pi_- - \Pi_0) \tag{3}$$

Note that values Π_-, Π_+ and Π_0 are calculated as the result of the integration over the whole body. We may have a small difference of large numbers if calculate $\Pi_+ - \Pi_-$ directly. It may give uncertain mistake in numerical calculation. The values $\Pi_\pm - \Pi_0$ can be calculated as a result of the integration over only the inclusion.

Given boundary conditions, we assume that the inclusion is in the phase state minus if $F > 0$ and in the phase state plus if $F < 0$. The condition $F = 0$ determines the transformation ("switch") surface in the space of external parameters which are the external deformations, the crack length, etc.

It can be shown [2-4] that

$$\Pi_- - \Pi_0 = \frac{1}{2}\int_V \mathbf{q}^- : \left(\mathbf{C}_1^-\right)^{-1} : \mathbf{q}_0^- \, dV \tag{4}$$

$$\Pi_+ - \Pi_0 = \int_V \left(\gamma_*^+ + \frac{1}{2}\mathbf{q}^+ : \left(\mathbf{C}_1^+\right)^{-1} : \mathbf{q}_0^+ \right) dV \tag{5}$$

where

$$\mathbf{q}_0^- = -\mathbf{C}_1^- : \boldsymbol{\varepsilon}^0, \quad \mathbf{q}^- = -\mathbf{C}_1^- : \boldsymbol{\varepsilon}^-, \quad \mathbf{q}_0^+ = \mathbf{C}_+ : \boldsymbol{\varepsilon}^p - \mathbf{C}_1^+ : \boldsymbol{\varepsilon}^0, \quad \mathbf{q}^+ = \mathbf{C}_+ : \boldsymbol{\varepsilon}^p - \mathbf{C}_1^+ : \boldsymbol{\varepsilon}^+, \tag{6}$$

$$\mathbf{C}_1^- = \mathbf{C}_- - \mathbf{C}_0, \quad \mathbf{C}_1^+ = \mathbf{C}_+ - \mathbf{C}_0,$$

$\varepsilon^+, \varepsilon^-$ are the strains inside the inclusion when it is in phase state minus or plus, respectively, V is the domain of the inclusion, ε^0 is the strain field in the domain V, if the body would be uniform,

$$\gamma_*^+ = \gamma + \frac{1}{2}\boldsymbol{\varepsilon}^p : \left(\mathbf{C}_+^{-1} - \mathbf{C}_0^{-1}\right)^{-1} : \boldsymbol{\varepsilon}^p \tag{7}$$

Thus, given boundary condition and the configuration of the body (the crack shape and length, relative position of the crack and the inclusion) the problem of the switch surface construction is reduced to the calculations of strains inside the domain of the inclusion when it is in different phase states and when there is no inclusion and a material in uniform.

Phase transformation of the inclusion in uniform external strain field. FEM procedure development and verification

For the simplicity sake we suppose that the materials are isotropic and study the case of plane strains, i.e. we consider a cylindrical inclusion with the axe m under uniform external strain field

$$\boldsymbol{\varepsilon}^0 = \varepsilon_1^0 \mathbf{e}_1 \otimes \mathbf{e}_1 + \varepsilon_2^0 \mathbf{e}_2 \otimes \mathbf{e}_2, \quad \mathbf{m} \perp \mathbf{e}_1, \mathbf{m} \perp \mathbf{e}_2 \tag{8}$$

We also assume that

$$\boldsymbol{\varepsilon}^p = \frac{\vartheta^p}{2}(\mathbf{I} - \mathbf{m} \otimes \mathbf{m}) \tag{9}$$

where I is the unit tensor.

Using the developed FEM procedure, we reproduced the results which were obtained earlier analytically. Typical domains of one-phase states of the inclusion and the switch surface are represented in the Fig. 2. Irrespective of the potential energy preferences, the inclusion can be in the "-" phase state if external strains are inside the grey area, while the hatched area corresponds to the "+" phase state. The thick line denotes the switch (transformation) surface $F = 0$.

For example, the inclusion can be only in "-" phase state if external strains belong the segment DE. When we reach the point E the "+" phase state becomes possible but the potential energy of the body with the inclusion in this state is greater the energy with the inclusion in the "-" phase state. After crossing the switch surface in the points F and C the "+" phase state of the inclusion becomes more preferable from the energy point of view.

The transformation surface can be closed or unclosed depending on the material parameters. It means that on some deformation paths phase transitions are not allowed whatever the values of strains are. Note that the location of the switch surface depends on the parameter γ, i.e. on the temperature. The switch surface can be moved to the undeformed state by changing the temperature and the inclusion will change the phase state without any external stress fields.

The correspondence between numerical and analytical results allow us to believe that the numerical procedures developed can be used successfully for more complicated problems of interaction between growing crack and localized structural transformations.

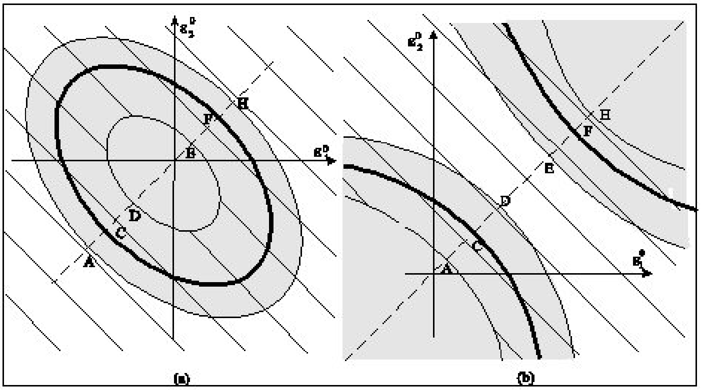

Figure 2: Switch surfaces in the case of plane deformation at various material parameters

Interaction between the crack and the phase-transforming inclusion

First, we calculated stresses and strains in a body with a crack and the inclusion (in the case of plane deformation). Strains inside the inclusion are not uniform in this case. The function F that determines the transformation surface depends on external strains and geometric parameters l, s, d (D =1) (see Fig.3) which characterize the sizes and the relative position of the crack and the inclusion. We studied in detail how the geometric parameters affect the possibility of the phase transformation and how critical strains and geometric parameters are related.

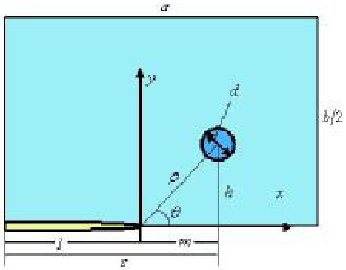

Figure 3: The crack and inclusion

The finite element grid is presented at fig.4.

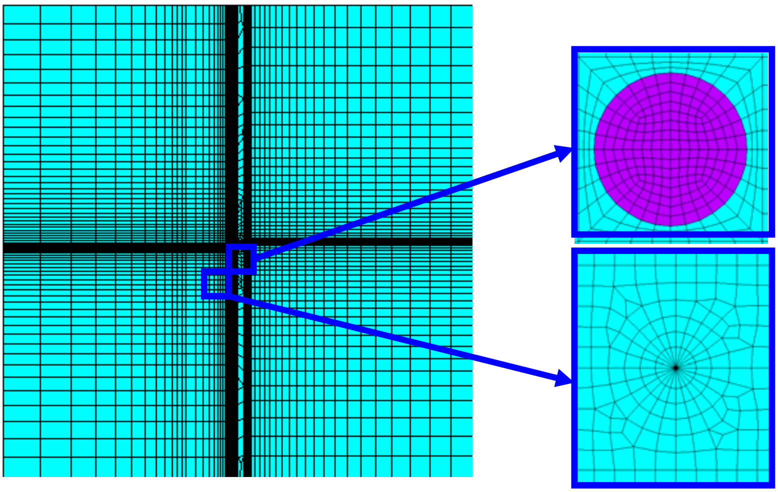

Fig.4: Finite element grid of the model

The example of the switch lines is represented in Fig. 5 for the case of uniaxial external deformation ε .

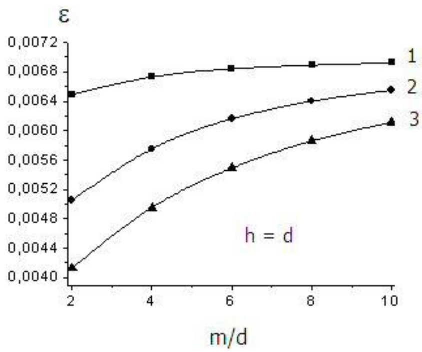

Figure 5: Interaction between the crack and phase transforming inclusion under uniaxial external stretching. The switch lines. 1- l/d=1, 2 – l/d = 6, 3 – l/d=10.

The crack path in dependence on the phase transforming inclusion

Now let us suppose that the crack is growing and determine the crack trajectory in the interrelation with the phase transformation in the inclusion. We assume that the crack grows according to the Parrish equation:

$$\Delta l = C \cdot \Delta K^{p} \cdot \Delta N, \quad \text{where} \quad C = 1.39 \cdot 10^{-11} \frac{\text{m}}{\text{cycle} \cdot (\text{MPa}\sqrt{\text{m}})^{p}}, \quad p = 3.09 \tag{10}$$

where ΔN is an appropriate number of cycles (is chosen).
To determine the direction of the crack growth we admit one of the widely used hypotheses [7] based on the following statements:

1. The crack grows from the tip in the radial direction
2. The crack grows perpendicularly to the direction of the maximal stress.

Then the angle θ_0 between new and old directions of the crack growth can be determined from the equation:

$$\frac{d\sigma_\theta}{d\theta}\bigg|_{\theta=\theta_0} = 0 \tag{11}$$

The above condition coincides with

$$\tau_{r\theta}(\theta = \theta_0) = 0 \tag{12}$$

This means that the crack propagates along the line of the principal stresses in the neighborhood of the crack tip.
Both stress intensity factors K_I and K_{II} are not zero in the case. The derivative of the tangential stress is given by the formula [6]:

$$\frac{d\sigma_\theta}{d\theta} = \frac{1}{\sqrt{2\pi r}}\left[K_I \cos^3\frac{\theta}{2} - \frac{3}{4}K_{II}\left(\sin\frac{\theta}{2} + 3\sin\frac{3\theta}{2}\right)\right] = 0 \tag{13}$$

Then from the condition (11) it follows that the angle θ_0 between the new and old directions of growth is given by

$$\theta_0 = \arcsin\frac{n}{\sqrt{9n^2+1}} - \arcsin\frac{3n}{\sqrt{9n^2+1}}, \quad \text{where} \quad n = \frac{K_{II}}{K_I} \tag{14}$$

One can see that the sign of the angle θ_0 depends on the sign of K_{II}: $\theta_0 < 0$ if $K_{II} > 0$ and $\theta_0 > 0$ if $K_{II} < 0$.

The possible trajectory of the crack is determined by the following steps. Initial stress intensity factors are determined from the static problem with the straight crack. The angle θ_0 between the new and old directions of crack growth is founded from (14). A small increment Δl is added to the crack length in the direction θ_0. The value of the increment Δl is founded from (10). Since the crack lengthening during one cycle is very small it was assumed that the crack grows in this direction during some fixed number of the cycles ΔN. Then static problem with a new geometry of the crack is solved and new values of the stress intensity factors are found. Then the process is repeated.

We have sketched above how to determine the trajectory of the crack growth. Now we are concentrating on the interconnection between the crack growth and phase transformation in the inclusion. One can choose the parameters of the problem so that the crack growth initiates the phase transformation in the inclusion.

Fig.6 presents the interaction between the phase transition and the growing crack. At this figure the inclusion becomes bigger, i.e. $\varepsilon^p > 0$

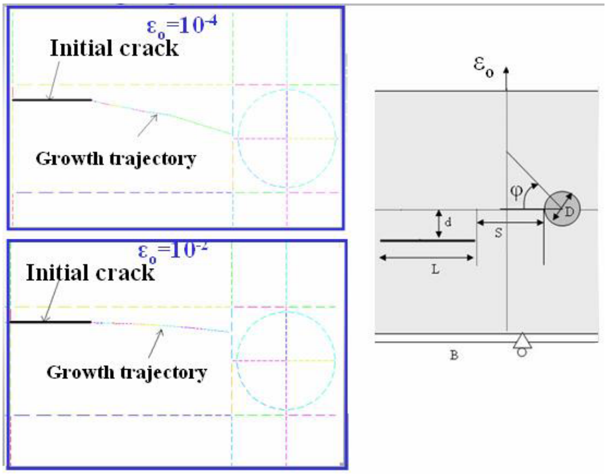

Fig.6: Interaction between the growing crack and phase transforming inclusion when $\varepsilon^p > 0$

One can see that phase transforming inclusion “attracts” the trajectory of the growing crack. It have to be mentioned that the increasing of the external field leads to the vanishing this effect of “attraction”

Fig.7 presents the interaction between the phase transition and the growing crack. At this figure the inclusion becomes smaller, i.e. $\varepsilon^p < 0$

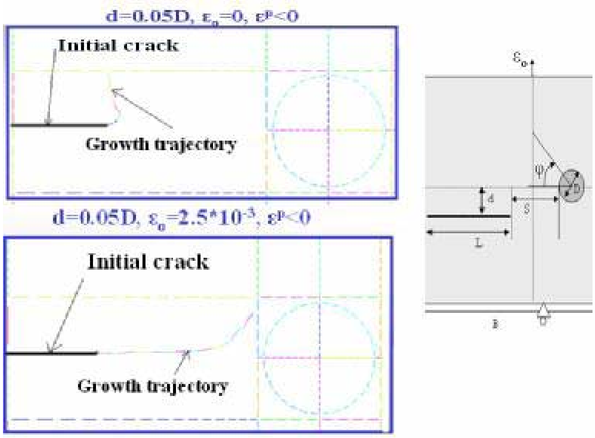

Fig.7: Interaction between the growing crack and phase transforming inclusion when $\varepsilon^p < 0$

One can see that phase transforming inclusion “repels” the trajectory of the growing crack. It have to be mentioned that the increasing of the external field leads to the vanishing this effect of “attraction”. This phenomena has a natural explanation if one imagine stresses around the inclusion after the phase transformation. The effect becomes weaker if the external strain increases.

It should be noted that the effects take place when the distance between the tip of the crack and the center of the inclusion is comparable with the diameter of the inclusion (at reasonable choice of the material parameters). This means impossibility of using asymptotic methods and gives additional reasons to develop numerical procedures.

Conclusions

– The crack can produce phase transformations in an inclusion (a grain) that in turn affects the trajectory of the crack.

– The phase transformation leads to the deviation of the crack trajectory towards or away from the inclusion, depending on materials parameters. The crack may “repels” the inclusion if the phase transformation is accompanied by the transformation strain ε^p such that tr ε^p is negative.

– There is a competition between external stress and crack-induced stress. Increasing of the external stress leads to the gradual decreasing of the crack trajectory deviation.

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