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Phase transition in a plastic layer: finite strains analytical solution

Problem on phase transition (PT) in a thin layer in a rigid-plastic half-space is solved at large strains. Thermodynamical theory of martensitic PT [1, 2] is applied. The nontrivial consequence of account for geometrical nonlinearities (even at small strains) is a definite transformation path, i.e. sequences of volumetric and shear transformation strain variation during the PT. Two mechanisms of experimentally observed positive effect of shear stresses on PT are found. The first one is related to necessity of fulfillment of the yield condition for the transforming material. The second mechanisms is connected with the transformation shear work. Greenwood–Jonson mechanism of transformation induced plasticity is modeled. The results obtained are in a qualitative agreement with known experiments.

1. Problem formulation

To simulate experimentally observed effect of shear stress and strain on PT let us consider an infinite rigid-plastic half-space with prescribed normal σ_n and shear τ stresses on the whole surface (Fig. 1) under plane strain condition. Assume that a coherent PT occurs in the layer along the whole surface and the solution does not depend on the x coordinate. For coherent PT displacements are continuous across the interface. Material outside of the layer is rigid. In Fig. 1, *a* transformed particle is shown after transformation strain, but to satisfy displacement continuity across the interface AB and independence of solution of x, additional plastic strain is needed (Fig. 1, *b*). We assume that total, transformation and plastic deformation gradients are homogeneous in a layer and stress field is homogeneous and time independent. At small strains the problem is solved in [3]. For simplicity we assume that at the beginning of the PT the yield stress makes an instantaneous jump to the value in the new phase. Complete system of equations is as follows [1, 2].

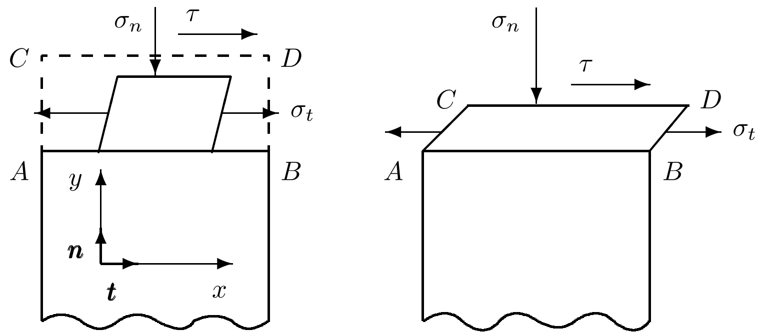

Fig. 1. Scheme of coherent SC in a thin layer

Decomposition of deformation gradient $\boldsymbol{F}$ into plastic $\boldsymbol{F}_p$ and transformational $\boldsymbol{F}_t$ parts

$$\boldsymbol{F} = \boldsymbol{F}_t \cdot \boldsymbol{F}_p \, . \tag{1}$$

Decomposition of deformation rate

$$\boldsymbol{d} := \left(\dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1}\right)_s = \left(\dot{\boldsymbol{F}}_t \cdot \boldsymbol{F}_t^{-1}\right)_s + \boldsymbol{d}_p \, ; \qquad \boldsymbol{d}_p := \left(\boldsymbol{F}_t \cdot \dot{\boldsymbol{F}}_p \cdot \boldsymbol{F}_p^{-1} \cdot \boldsymbol{F}_t^{-1}\right)_s \, . \tag{2}$$

Tresca yield condition for the transforming layer and associated flow rule

$$\varphi(\boldsymbol{T}) = 2\,(\boldsymbol{S} : \boldsymbol{S}) = (\sigma_n - \sigma_t)^2 + 4\,\tau^2 - \sigma_y^2 = 0 \, ; \qquad \boldsymbol{S} := dev\,\boldsymbol{T} \, ; \tag{3}$$

$$\boldsymbol{d}_p = d_{pn}\,(\boldsymbol{n}\boldsymbol{n} - \boldsymbol{t}\boldsymbol{t}) + \hat{\gamma}_p\,(\boldsymbol{t}\boldsymbol{n})_s = 2\,h\,\boldsymbol{S} \, ; \qquad d_{pn} = h\,(\sigma_n - \sigma_t) \, ; \qquad \hat{\gamma}_p = 4\,h\,\tau \, . \tag{4}$$

PT criterion and extremum principle

$$X := \int_{\boldsymbol{i}}^{\boldsymbol{F}_{t2}} \frac{\rho_1}{\rho}\,\boldsymbol{T} : \left(d\boldsymbol{F}_t \cdot \boldsymbol{F}_t^{-1}\right) h_1 - \rho_1\,\Delta\psi(\theta)\,h_1 = \rho_1\,k\,h_1 + 2\,E \, ; \tag{5}$$

$$\int_{\boldsymbol{i}}^{\boldsymbol{F}_{t2}} \frac{\rho_1}{\rho^*}\,\boldsymbol{T}\boldsymbol{:}\left(d\,\boldsymbol{F}_t^*\cdot\boldsymbol{F}_t^{-1\,*}\right)\,h_1^*\;-\;\rho_1\,\Delta\,\psi\,h_1^*\;-\;2\,E\;-\;\rho_1\,k\,h_1^*\;\;\rightarrow\;\;max\,. \qquad (6)$$

Here $\boldsymbol{T}$ is the Cauchy stress and σ_t the tangential stress, σ_y the yield limit at simple compression; X the driving force for PT; k the experimentally determined value of dissipation increment due to PT; $\Delta\,\psi\,(\theta)$ the difference in thermal part of free energy of phases; θ the temperature; ρ_1 the mass density of phase 1 (before PT); h_1 the thickness of transforming layer in the reference configuration; E the the surface energy increment; ρ the current variable mass density in the course of PT; $\boldsymbol{i}$ is the two dimensional unit tensor.

2. Phase transition condition

PT will be considered as a process of variation of the transformation deformation gradient from the initial $\boldsymbol{F}_{t1}\;=\;\boldsymbol{i}$ to final $\boldsymbol{F}_{t2}$ value which is accompanied by a jump in all thermomechanical properties. Let us consider the kinematics of the problem. The deformation gradient in the layer has the following form $\boldsymbol{F}\;=\;\boldsymbol{i}\,+\,\gamma\,\boldsymbol{tn}\,+\,\delta\,\boldsymbol{nn}$, where δ and γ are the normal and shear strains, $\boldsymbol{n}$ and $\boldsymbol{t}$ are the unit vectors in directions x and y correspondingly. Direct calculations results in

$$\dot{\boldsymbol{F}}\;=\;\dot{\gamma}\,\boldsymbol{tn}\,+\,\dot{\delta}\,\boldsymbol{nn}\,;\qquad \boldsymbol{F}^{-1}\;=\boldsymbol{i}\,-\,\frac{\gamma}{1+\delta}\,\boldsymbol{tn}\,-\,\frac{\delta}{1+\delta}\,\boldsymbol{nn}\,;\qquad \boldsymbol{d}\;=\;\left(\dot{\boldsymbol{F}}\right)_s\,\frac{1}{1+\delta}\,. \quad (7)$$

For the transformation deformation gradient we accept the following expression $\boldsymbol{F}_t=a\,\boldsymbol{i}+\gamma_t\,\boldsymbol{tn}$, where $a=1+\varepsilon$ and γ_t are the normal and shear transformation strains. Direct calculations allows to obtain

$$\boldsymbol{F}_t^{-1}\;=\;\frac{1}{a}\,\boldsymbol{i}\,-\,\frac{\gamma_t}{a^2}\,\boldsymbol{tn}\,;\qquad \dot{\boldsymbol{F}}_t\;=\;\dot{a}\,\boldsymbol{i}\,+\,\dot{\gamma}_t\,\boldsymbol{tn}\,;\qquad \boldsymbol{d}_t\;=\;\frac{1}{a}\left(\dot{a}\,\boldsymbol{i}\,+\,\left(\dot{\gamma}_t\,-\,\frac{\dot{a}\,\gamma_t}{a}\right)\,(\boldsymbol{tn})_s\right)\,. \quad (8)$$

Calculating work integral in PT criterion (5) with account for $\boldsymbol{T}\;=\;\boldsymbol{const}$, we obtain

$$A_t\;:=\;\int_{\boldsymbol{i}}^{\boldsymbol{F}_{t2}}\frac{1}{\rho}\,\boldsymbol{T}\boldsymbol{:}d\,\boldsymbol{F}_t\cdot\boldsymbol{F}_t^{-1}\;=\;\frac{1}{\rho_1}\left(0.5\,(\sigma_n\,+\,\sigma_t)\left(a_2^2\,-\,1\right)\,+\,\tau\,a_2\,\gamma_{t2}\,-\,2\,\tau\int_1^{a_2}\gamma_t\,d\,a\right)\,. \quad (9)$$

It is evident that two first terms in Eq. (9) are transformation path independent, but the last term depends in which sequences γ_t and a vary during the transformation process. To determine the actual transformation path, the extremum principle (6) will be used, which at $\tau\,\geq\,0$ results in

$$P\;:=\;\int_1^{a_2}\gamma_t\,d\,a\;\;\rightarrow\;\;min \qquad\qquad \text{or} \qquad\qquad P\;:=\;\int_0^{\varepsilon_2}\gamma_t\,d\,\varepsilon\;\;\rightarrow\;\;min\,. \qquad (10)$$

Here $\gamma_t\,\geq\,0$ (as the signs of τ and γ_t coincide). Let us consider two cases.

1. $\varepsilon\,\geq\,0$, transformational dilatation. The minimum value of $P=0$ (as both γ_t and $\varepsilon\,\geq\,0$), can be reached by the following process : first, at $\gamma_t=0$, ε grows to final value ε_2, then at $\varepsilon\,=\,\varepsilon_2$ γ_t grows to γ_{t2}.
2. $\varepsilon\,\leq\,0$. The minimum value of P corresponds to the following transformation process : first, at $\varepsilon=0$, γ_t increases to its maximum value γ_{t2}, then at $\gamma_t\,=\,\gamma_{t2}$ ε decreases to ε_2.

In this case $P\;:=\;\gamma_{t2}\,\varepsilon_2\;=\;-\,\gamma_{t2}\;\mid\varepsilon_2\mid$. For both cases PT criterion (5) has the following form

$$\left(\frac{1}{2}\,(\sigma_n\,+\,\sigma_t)\left(a_2^2\,-\,1\right)\,+\,\mid\tau\,\gamma_{t2}\mid\;(1+\mid\varepsilon_2\mid)\right)h_1\,-\,\rho_1\,\Delta\,\psi\,(\theta)\;h_1\;=\;\rho_1\,k\,h_1\,+\,2\,E\,. \; (11)$$

At small strain formulation the solution of this problem is path independent and consequently the transformation path is undetermined. But if we start with the exact at finite strain Eq. (11), then even at infinitesimal ε_2 and γ_{t2} we obtain new phenomenon, namely definite transformation path. Consequently, strict geometrically nonlinear formulation is important even at small strains.
Let us determine the thickness of the layer, based on the extremum principle (6). Assume that k depends on volume fraction of new phase $\dfrac{h_1}{L}$, where L is the final thickness of the layer. Maximizing $(A_t-\Delta\,\psi\,(\theta)-k)\,\rho_1\,h_1-2\,E$ with respect to h_1 we obtain $A_t-\Delta\,\psi\,(\theta)-\,k-\,\dfrac{\partial\,k}{\partial\,h_1}\,h_1\;=\;0$, or taking into account Eq. (11) $2\,E\;=\;\dfrac{\partial\,k}{\partial\,h_1}\,\rho_1 h_1^2$.
For linear $k\;=\;A\,+\,B\,h_1/L\;\;(B>0)$ we get $h_1\;=\;\left(\dfrac{2\,E\,L}{\rho_1\,B}\right)^{1/2}$.

From the yield condition (3) it follows $\sigma_t = \sigma_n - \frac{\varepsilon}{|\varepsilon|}\sqrt{\sigma_{y2}^2 - 4\tau^2}$. We took into account that at $\varepsilon > 0$ plastic tension in direction $\boldsymbol{n}$ is possible at $\sigma_n > \sigma_t$ only; at $\varepsilon < 0$ plastic compression in direction $\boldsymbol{n}$ is possible at $\sigma_n < \sigma_t$ only. Substituting σ_t in Eq. (11) we obtain the PT pressure

$$\sigma_n = K + 0.5\,\frac{\varepsilon}{|\varepsilon|}\sqrt{\sigma_{y2}^2 - 4\tau^2} - |\tau|\, M\,, \tag{12}$$

$$K := \frac{\rho_1\,\Delta\psi(\theta) + \rho_1\,k + E/h_1}{a_2^2 - 1}\,; \qquad M := |\gamma_{t2}|\,\frac{(1 + |\varepsilon_2|)}{a_2^2 - 1}\,. \tag{13}$$

Let us analyze the results obtained for the case $\varepsilon > 0$. The increase of τ *decreases* the PT pressure, which is in agreement with experiments (see [3, 4] and references). Maximal decrease is equal to $0.5\,\sigma_{y2}\,(1+M)$ at $\tau = 0.5\,\sigma_{y2}$. It follows from Eq.(12) that shear stresses promote the PT condition by two mechanisms. First, τ contributes to the yield condition of the second phase and PT criterion (12) in a way equivalent to the *decrease* of the yield limit of the second phase. This mechanisms acts even at $\gamma_t = 0$. The second way is related to the transformation shear work. At large γ_{t2} and maximum possible $\tau = 0.5\,min\,(\sigma_{y2}, \sigma_{y1})$ the term $\tau_{max}\,M$ can exceed the term $\frac{\rho_1\,k + E/h_1}{a_2^2 - 1}$ in Eq. (12) and PT will occur under pressure which is less than thermodynamic equilibrium pressure $\sigma_{n,eq} := \frac{\rho_1\,\Delta\psi}{a_2^2 - 1}$, which corresponds to the results obtained in some experiments [4].

The interface propagation can be modeled as a subsequent nucleation in the layer contacting the existing layer of the second phase. For rigid–plastic material stress variation in each subsequent layer is the same as in the first one. Consequently, the interface propagation criterion has the same form, as the nucleation criterion (11). As the area of interface is constant during the interface motion, then the increment of surface energy is zero. As the increment of surface energy disappear immediately after appearance of the nucleus, then at fixed stresses and temperature the layer thickness h_1 will increase to the value h at which the threshold k will be equal to the driving force X at the nucleation. This condition results in

$$X = \rho_1\,k\,(h_1) + \frac{2\,E}{h_1} = \rho_1\,k\,(h)\,. \tag{14}$$

For linear function $k\,(h_1)$ we obtain $h = h_1 + \frac{2\,E\,L}{\rho_1\,B\,h_1} = 2\,h_1$, i.e. due to spontaneous interface propagation the thickness of layer becomes two times higher. Differentiating Eq. (12) at $E = 0$ with respect to time, we obtain evolution equation for h_1 at variable stresses and temperature.

3. Integration of flow rule

Plastic deformation gradient can be calculated as

$$\boldsymbol{F}_p = \boldsymbol{F}_t^{-1}\cdot\boldsymbol{F} = \frac{1}{a}\left(\boldsymbol{i} + \delta\,\boldsymbol{n}\boldsymbol{n} + \left(\gamma - \frac{\gamma_t}{a}\,(1+\delta)\right)\boldsymbol{t}\boldsymbol{n}\right)\,. \tag{15}$$

It follows from the plastic incompressibility condition

$$det\,\boldsymbol{F}_p = \frac{1+\delta}{a^2} = 1 \qquad \Longrightarrow \qquad \delta = a^2 - 1\,; \qquad a = \sqrt{1+\delta}\,. \tag{16}$$

It is convenient to derive expression for the plastic deformation rate using Eq. (2)

$$\boldsymbol{d}_p = \left(\dot{\boldsymbol{F}}\cdot\boldsymbol{F}^{-1}\right)_s - \left(\dot{\boldsymbol{F}}_t\cdot\boldsymbol{F}_t^{-1}\right)_s = d_{pn}\,(\boldsymbol{n}\boldsymbol{n} - \boldsymbol{t}\boldsymbol{t}) + \hat{\gamma}_p\,(\boldsymbol{t}\boldsymbol{n})_s\,; \tag{17}$$

$$\text{with} \qquad d_{pn} = \frac{\dot{a}}{a} \qquad \text{and} \qquad \hat{\gamma}_p = \frac{1}{a}\left(\frac{\dot{\gamma}}{a} - \dot{\gamma}_t + \frac{\dot{a}}{a}\,\gamma_t\right) \tag{18}$$

for the normal and shear components of plastic deformation rate. Combining equations (4), $(18)_1$ and yield condition we obtain

$$\hat{\gamma}_p = 4\,h\,\tau = 4\,\frac{\dot{a}}{a}\,\frac{\tau}{(\sigma_n - \sigma_t)} = 4\,\frac{\dot{a}}{a}\,\frac{\tau}{\sqrt{\sigma_{y2}^2 - 4\tau^2}}\,\frac{\varepsilon}{|\varepsilon|}\,. \tag{19}$$

It is clear, that plastic strain occurs when volumetric transformation strain varies only. Let us determine shear strain γ by integrating of Eq. $(18)_2$ with account for Eq. (19). We should distinguish two cases.
1. $\varepsilon \geq 0$. First, ε grows at $\gamma_t = 0$. Then

$$\hat{\gamma}_p = \frac{\dot{\gamma}}{a^2} = 4\,\frac{\dot{a}}{a}\,\frac{\tau}{\sqrt{\sigma_{y2}^2 - 4\,\tau^2}} \qquad \text{and} \qquad \gamma = 2\left(a^2 - 1\right)\frac{\tau}{\sqrt{\sigma_{y2}^2 - 4\,\tau^2}}\,. \quad (20)$$

Second, at $a = a_2$ γ_t grows. We have

$$\hat{\gamma}_p = \frac{1}{a_2}\left(\frac{\dot{\gamma}}{a_2} - \dot{\gamma}_t\right) = 0 \quad (\text{as } \dot{a} = 0) \quad \text{and} \quad \gamma = 2\left(a_2^2 - 1\right)\frac{\tau}{\sqrt{\sigma_{y2}^2 - 4\,\tau^2}} + a_2\,\gamma_t\,. \quad (21)$$

2. Case $\varepsilon \leq 0$ is considered similarly. For both cases after the finishing the PT

$$\gamma_2 = (1 + \mid \varepsilon_2 \mid)\,\gamma_{t2} + 2 \mid a_2^2 - 1 \mid \frac{\tau}{\sqrt{\sigma_{y2}^2 - 4\,\tau^2}} := \tilde{\gamma}_t + \tilde{\gamma}_p\,. \quad (22)$$

Expression (22) for shear strain consist of transformational (first term) and plastic (second term) parts. Plastic flow occurs at arbitrary (even at infinitesimal) shear stresses, external stresses τ and σ_n must not satisfy the yield condition. Plastic straining takes place due to variation of volumetric transformation strain. Such phenomenon is called transformation induced plasticity or TRIP [5]. This problem models the well–known mechanism of TRIP due to Greenwood–Jonson effect. Relation (22) describes qualitatively good known experimental relationship between the external stresses and plastic strain [5].
Based on Eq. (22) we can express the shear stress in terms of plastic shear and substitute this dependence in PT criterion (12). We obtain

$$\sigma_n = K + \frac{\sigma_{y2}}{2}\,\frac{\varepsilon}{\mid \varepsilon \mid}\,\frac{\left(a_2^2 - 1\right)}{\sqrt{\left(a_2^2 - 1\right)^2 + \tilde{\gamma}_p^2}} - \frac{\sigma_{y2}}{2}\,\frac{\mid \tilde{\gamma}_p \mid}{\sqrt{\left(a_2^2 - 1\right)^2 + \tilde{\gamma}_p^2}}\,M\,. \quad (23)$$

Eq. (23) exhibits the experimentally observed [3, 4] decrease of PT pressure under the growing plastic shear; at $2\,\tau = \sigma_{y2}$ $\tilde{\gamma}_p \to \infty$ and second term in Eq. (23) disappears.

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