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PHASE TRANSITIONS IN ELASTOPLASTIC MATERIALS: CONTINUUM THERMOMECHANICAL THEORY AND EXAMPLES OF CONTROL. PART II

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ABSTRACT

The thermomechanical theory of phase transitions (PT) developed by Levitas (Part I of the paper) is extended to the case with displacement discontinuities across an interface (noncoherence and fracture). Two boundary-value problems are solved analytically: the appearance of a spherical nucleus in an infinite elastoplastic sphere under applied pressure (without or with interfacial fracture) with application to temperature-induced PT in steel and pressure-induced PT graphite–diamond; noncoherent PT in a rigid–plastic half-space. The effect of strain hardening on the PT condition is discussed. The experimental phenomena described in the paper are enumerated. Results of the numerical modelling of the technological process of diamond synthesis are discussed in connection with the explanation of experimental results and revelation of the pressure self-regulation effect. Some methods for the control of PT by means of the purposeful control of stress–strain fields are suggested, using analysis of various useful examples of stress field variation during PT in the problems solved in Parts I and II. © 1997 Elsevier Science Ltd

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1. INTRODUCTION

In this part of the paper the following problems are considered. The thermomechanical theory developed in Part I is extended to the case with displacement discontinuities across an interface (noncoherence and fracture). It is assumed that PT and fracture (or noncoherence) criteria are mutually independent, and these processes are coupled through the stress fields only. Growing transformation strain generates the stresses, which are necessary for fracture (sliding along the interface), and fracture (noncoherence) changes the stress variation in the transforming particle. Two boundary-value problems are formulated and solved analytically:

- the appearance of a spherical nucleus in an infinite elastoplastic sphere under applied pressure (without or with interfacial fracture) with application to temperature-induced PT in steel and pressure-induced PT graphite–diamond;
- noncoherent PT in a rigid-plastic half-space.

The PT criterion has the form

$$\int_{V_n} X\,\mathrm{d}V_n = \int_{V_n}\int_{\varepsilon_1^t}^{\varepsilon_2^t} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}^t\,\mathrm{d}V_n + \Delta\psi^\theta V_n = kV_n, \quad k = L\sigma_y\varepsilon_o \tag{1}$$

for the first problem (elastic properties of parent and product phases are the same) and the form

$$\int_t^{t+\Delta t}\int_{\Sigma_n} \mathbf{p}\cdot\mathbf{v}\,\mathrm{d}\Sigma_n\,\mathrm{d}t = (\Delta\psi^\theta + k)V_n \tag{2}$$

for the second problem [see (7) and (11) in Levitas (1997)]. Here X is the driving force for PT, V_n and Σ_n are the volume and surface of the nucleus, $\boldsymbol{\sigma}$ and $\mathbf{p} = \boldsymbol{\sigma}\cdot\mathbf{n}$ are the stress tensor and vector, respectively, $\mathbf{n}$ is the unit normal to Σ_n, $\Delta\psi^\theta = \rho(\psi_2^\theta - \psi_1^\theta)$ is the difference of the thermal parts of the free energy, $\boldsymbol{\varepsilon}^t$ and ε_0 are the transformation strain tensor and its volumetric part, k is the dissipation due to PT, σ_y is the yield stress, t is the time and $\mathbf{v}$ is the velocity of points Σ_n from the side of the nucleus. In the second problem the volume V_n contains the transformation strain only, and (2) follows from (1) and the Gauss theorem. Assume the following explicit expression for the thermal part of the free energy (Huo and Müller, 1993):

$$\psi_i^\theta = \psi_{oi} - s_{oi}(\theta-\theta_o) - \nu_i\theta(\ln\theta/\theta_o - 1) - \nu_i\theta_o, \quad i = 1, 2. \tag{3}$$

Here $\nu_i > 0$ are the specific heats, s_{oi} and ψ_{oi} are constants. In the case of small $(\theta/\theta_0 - 1)$ we have $\ln\theta/\theta_0 \simeq \theta/\theta_0 - 1$. It is possible to choose the reference temperature from the condition $\Delta\psi^\theta(\theta_0) = 0$, so that $\Delta\psi_0 = 0$. Then

$$\Delta\psi^\theta = -\rho\Delta s_o(\theta-\theta_o) - \frac{\rho\Delta\nu}{\theta_o}(\theta-\theta_o)^2. \tag{4}$$

Then some results of the numerical modelling of the technological process of diamond synthesis are discussed in connection with the explanation of experimental results and revelation of the so-called pressure self-regulation effect. In Section 4 some methods of control of the PT by means of the purposeful control of stress–strain fields are suggested, using analysis of various useful examples of stress field variation during PT in the problems solved.

We assume for convenient that compressive stresses and strains are positive (except in Section 2.2).

2. APPEARANCE OF A SPHERICAL NUCLEUS IN AN INFINITE ELASTOPLASTIC SPHERE

2.1. *Phase transition criterion*

Let us consider the PT in a spherical inclusion with radius R in an infinite elasto–perfectly plastic sphere under applied external pressure p [Fig. 1(a)]. Elastic properties of parent and new phases are the same, $\boldsymbol{\varepsilon}^t = \frac{1}{3}\varepsilon_0\mathbf{I}\xi$, where ξ is the parameter, growing from 0 to 1 during the PT. Then the pressure $\tilde{p}$ in a nucleus is determined by formulas (Roitburd and Temkin, 1986; Fischer *et al.*, 1994):

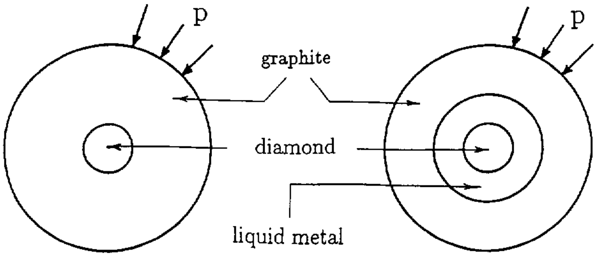

Fig. 1. Appearance of a spherical nucleus in an elastoplastic sphere in a general case and for the problem of PT graphite–diamond.

$$\text{in the elastic region}\quad \tilde{p}_e = p - \frac{\varepsilon_o}{3C}, \quad |\varepsilon_o| \leqslant |\varepsilon_o'|, \quad \varepsilon_o' := 2\sigma_y C, \tag{5}$$

$$\text{in the plastic region}\ \tilde{p}_p = p - \frac{2}{3}\sigma_y\left(\ln\frac{\varepsilon_o}{2\sigma_y C} + 1\right), \quad |\varepsilon_o| > |\varepsilon_o'|. \tag{6}$$

Here $C = 3(1-\nu_0)/2E$, E is Young's modulus, ν_o is Poisson's ratio, σ_y is the yield stress of parent phase and ε_o' is the strain corresponding to the onset of plastic flow in the parent phase. Note that σ_y can be *positive* or *negative* and due to the condition $\varepsilon_0/(2\sigma_y C) > 0$ the signs of σ_y and ε_o *coincide*. Calculation of the work integral yields

$$\int_{\boldsymbol{\varepsilon}^{t1}}^{\boldsymbol{\varepsilon}^{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}^t = \int_0^{\varepsilon_o} \tilde{p}\,\mathrm{d}\varepsilon_o = \int_0^{\varepsilon_o'} \tilde{p}_e\,\mathrm{d}\varepsilon_o + \int_{\varepsilon_o'}^{\varepsilon_o} \tilde{p}_p\,\mathrm{d}\varepsilon_o = p\varepsilon_o - A_m \tag{7}$$

with

$$A_m := \frac{2}{3}\sigma_y\varepsilon_o\left(\frac{\sigma_y C}{\varepsilon_o} + \ln\frac{\varepsilon_o}{2\sigma_y C}\right) \tag{8}$$

during elastoplastic deformation and

$$\int_{\boldsymbol{\varepsilon}^{t1}}^{\boldsymbol{\varepsilon}^{t2}} \boldsymbol{\sigma} : \mathrm{d}\boldsymbol{\varepsilon}^t = p\varepsilon_o - \frac{\varepsilon_o^2}{6C} \tag{9}$$

during elastic deformation. Substituting (7) and (9) in (1) we obtain the PT pressure in the elastoplastic and elastic region, respectively:

$$p = \frac{2}{3}\sigma_y\left(\frac{\sigma_y C}{\varepsilon_o} + \ln\frac{\varepsilon_o}{2\sigma_y C}\right) + \frac{1}{\varepsilon_o}\left(k - \rho\Delta s_o(\theta - \theta_o) - \frac{\rho\Delta v}{\theta_o}(\theta - \theta_o)^2\right), \tag{10}$$

$$p = \frac{\varepsilon_o}{6C} + \frac{1}{\varepsilon_o}\left(k - \rho\Delta s_o(\theta - \theta_o) - \frac{\rho\Delta v}{\theta_o}(\theta - \theta_o)^2\right). \tag{11}$$

Equations (10) and (11) at $k = 0$ coincide with the corresponding equations in the paper by Roitburd and Temkin (1986) and differ from equations obtained by Fischer *et al.* (1994). Adiabatic heating is taken into account by Levitas (1996a).

For the description of PT progress we can consider the appearance of a new martensitic nucleus in an austenite+martensite mixture. In the first approximation, neglecting the energy of internal stresses in a mixture and assuming $\sigma_y = c\sigma_{yM} + (1-c)\sigma_{yA}$, where c is the volume fraction of martensite, σ_{yA} and σ_{yM} are the yield stresses of austenite and martensite, we can use (8) and (10). As for steels, σ_{yM} is several times σ_{yA}, so the PT pressure should be increased with increase in the martensite fraction.

A significant increase in σ_{yA} and σ_{yM} (we omit the sign $|\ldots|$) with the temperature decrease should also be taken into account. But the growth of A_m and p with growing σ_y is limited by the condition $|\varepsilon_o| \leqslant |\varepsilon_o'| := 2|\sigma_y|C$, i.e. until $\sigma_y = \varepsilon_o'/2C$ (at $C = 5 \times 10^{-4}$ MPa^{-1} $\sigma_y = \varepsilon_o' \times 10^5$ MPa). At larger σ_y the material is deformed elastically and $A_m = \varepsilon_o^2/6C$ (at $C = 5 \times 10^{-4}$, $A_m = \varepsilon_o^2 \cdot 10^5/3$ is independent of the yield stress. In the example below (at $C = 5 \times 10^{-4}$, $\varepsilon_o = 0.026$) the material is deformed plastically until $\sigma_y = 2.6 \times 10^3$ MPa and the maximum value of $A_m = 22.53$ MPa, i.e. the value of the mechanical work, is increased very little in comparison with the value $A_m = 20.576$ MPa at $\sigma_y = 10^3$ MPa.

2.2. *Temperature-induced PT in steel*

In this section it is convenient to consider tensile strains and stresses as positive. For temperature-induced PT, $p = 0$, $\theta = \mathrm{M_s}$, where M_s is the martensite start temperature which can be determined from (10) and (11). To estimate the value of k and compare it with the mechanical work A_m let us use the material parameters for steel Fe+30% Ni from the paper by Kaufman and Cohen (1958) (see also Fischer *et al.*, 1994):

$$\Delta\psi^\theta = a(\theta-\theta_o)+b(\theta-\theta_o)^2,$$

$$a = -\rho\Delta s_o = 0.904\,\mathrm{MPa\,K^{-1}}, \quad b = -\rho\frac{\Delta v}{\theta_o} = -3.356\times 10^{-4}\,\mathrm{MPa\,K^{-2}},$$

$$M_s = 220\,\mathrm{K}, \quad \theta_o = 440\,\mathrm{K}, \quad \Delta\psi^\theta(M_s) = -215.12\,\mathrm{MPa},$$

$$\varepsilon_o = 0.026, \quad E = 2.1\times 10^5\,\mathrm{MPa}, \quad \nu_o = 0.3, \quad \sigma_y = 10^3\,\mathrm{MPa}. \tag{12}$$

The value σ_y for austenite is overestimated considerably. Even in this case $A_m = 20.576$ MPa and the value k is determined from (10) at $p = 0$ is $k = 194.554$ MPa, i.e. 9.455 times larger than A_m. The coefficient L in (1) is also very high: $L = 7.48$.

There is an opinion (Estrin, 1993) that the very high value of $\Delta\psi^\theta(M_s)$ (and the difference $M_s - \theta_o$) typical of PT in steels is connected with the elastoplastic work during the PT due to relatively large ε_o. Our semiquantitative estimations show that the main reason for large $M_s - \theta_o$ lies mostly in large k. Allowance for adiabatic heating and plastic work in the process of self-accommodation of transformation shears can reduce the value of k.

The values of σ_y and k grow intensively with increasing c and decreasing θ. When k and σ_y are large enough, the temperature θ determined from (10) at $p = 0$, can be less than 0 K. This means that some residual austenite cannot be transformed into martensite due to cooling, which is in agreement with experiments for steels.

To determine the PT temperature explicitly, assume (Bell, 1973)

$$\sigma_{yA}(\theta) = \sigma_{yA}(0)\left(1-\frac{\theta}{\theta_{mA}}\right), \quad \sigma_{yM}(\theta) = \sigma_{yM}(0)\left(1-\frac{\theta}{\theta_{mM}}\right), \tag{13}$$

where θ_m is the melting temperature (θ_{mM} is a fitting parameter), but we neglect the temperature dependence of $\sigma_y C$. Designating $x = \theta - \theta_o$ we obtain

$$\begin{aligned}\sigma_y &= (1-c)\sigma_{yA} + c\sigma_{yM} = [(1-c)\sigma_{yA}(\theta_o) + c\sigma_{yM}(\theta_o)] \\ &\quad - x\left[(1-c)\frac{\sigma_{yA}(0)}{\theta_{mA}} + c\frac{\sigma_{yM}(0)}{\theta_{mM}}\right] = F(c) - M(c)x \end{aligned} \tag{14}$$

with

$$F(c) = (1-c)\sigma_{yA}(\theta_o) + c\sigma_{yM}(\theta_o) > 0$$

and

$$M(c) = (1-c)\frac{\sigma_{yA}(0)}{\theta_{mA}} + c\frac{\sigma_{yM}(0)}{\theta_{mM}} > 0 \tag{15}$$

(as $\varepsilon_o < 0$). Equation (10) leads to

$$p = \frac{2}{3}(F - Mx)B + L(F - Mx) - \frac{\rho \Delta s_o}{\varepsilon_o}x - \frac{\rho \Delta v}{\varepsilon_o \theta_o}x^2, \tag{16}$$

where

$$B = \frac{\sigma_y C}{\varepsilon_o} + \ln\frac{\varepsilon_o}{2\sigma_y C} > 0$$

does not depend on temperature. For a temperature-induced PT, $p = 0$ and

$$rx^2 + nx + m = 0, \tag{17}$$

where

$$r = \frac{\rho \Delta v}{\varepsilon_o \theta_o}, \quad n = \frac{\rho \Delta s_o}{\varepsilon_o} + \left(L + \frac{2}{3}B\right)M, \quad m = -F\left(L + \frac{2}{3}B\right) < 0. \tag{18}$$

The solution of (17) reads

$$x = -\frac{n}{2r} \pm \frac{\sqrt{n^2 - 4rm}}{2r}. \tag{19}$$

The sign "+" or "−" should be chosen from the condition $x = 0$ at $\sigma_{yA} = \sigma_{yM} = m = 0$, because at $\sigma_{yA} = \sigma_{yM} = 0$ the PT occurs at the equilibrium temperature $\theta = \theta_o$. It follows from the equation $-n \pm |n| = 0$, that for $n > 0$ we should use + sign and for $n < 0$ the − sign is valid. For $r > 0$ (i.e. $\Delta v > 0$), (19) always has a solution. What is more interesting is the case $r < 0$ (i.e. $\Delta v < 0$). It follows from (19) that PT proceeds (i.e. c grows) until

$$n^2 = 4rm \quad \text{and} \quad x = -\frac{n}{2r}. \tag{20}$$

It is evident from (19), that at $r < 0$, the value $x < 0$ at $n < 0$ only.

If there is additional cooling, (19) has no solution, because the PT stimulus $\Delta\psi^0$ grows more slowly than the resistance to PT $A_m + k$. This means that PT is impossible at a temperature less than some critical one, which is also in agreement with experiments at $\Delta v < 0$ (Estrin, 1993). The temperature $M_f = \theta_0 - n/2r$ is the martensite finish temperature. Note that usually the following explanation for the existence of M_f is used (Estrin, 1993): at low temperatures the growth of the PT stimulus becomes slow, but the yield stress increases intensively. As the resistance to PT in this case is related to the plastic straining only, then the PT is finished when the PT stimulus becomes smaller than the plastic resistance. As was shown above, the role of plastic resistance is overestimated by Estrin (1993).

2.3. *Phase transition graphite–diamond*

Let us consider PT graphite (G)–diamond (D), which is accompanied by a 54% volume decrease. The equilibrium pressure–temperature line calculated with the methods of chemical thermodynamics (Kurdyumov, 1980; Novikov *et al.*, 1987; Bundy, 1989) is shown in Fig. 2; this means that pressure and temperature variations, plastic straining and dissipation due to PT are neglected. The equilibrium line can be approximated by the equation (Kurdyumov, 1980; Novikov *et al.*, 1987; Bundy, 1989)

$$p_{eq} = 1.2575 + 0.0025\theta = a + b\theta (\text{GPa}). \tag{21}$$

In reality,

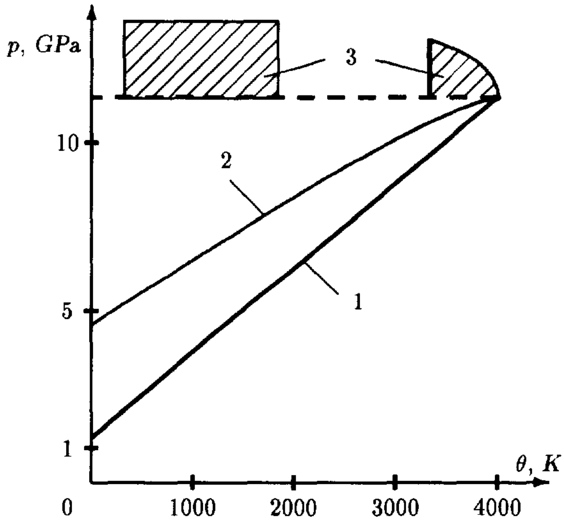

Fig. 2. Phase transition *G–D* diagram: 1—equilibrium line (Eq. (21)); 2—calculated curve (Eq. (23) at $k = 0$); 3—regions of the direct *G–D* PT (Bundy, 1989, experiments).

- solid–solid martensitic PT G–D proceeds at a pressure that is several times higher (Bundy, 1989) (Fig. 2);
- if PT occurs in the presence of some liquid metal [e.g. Fe, Ni, Co, NiMn (Novikov *et al.*, 1987)], then the PT can proceed at equilibrium pressure.

There are a number of physico-chemical theories which try to explain these phenomena qualitatively assuming some special chemical reactions, catalytic properties of metals or their properties as solvent metals, and so on (Kurdyumov, 1980; Novikov *et al.*, 1987). All of them may be correct, but first of all PT should be possible from the point of view of continuum thermodynamics. It will be shown that the above thermodynamic continuum theory allows us to explain both experimental results mentioned without any additional physical or chemical hypothesis.

Let us consider the appearance of a D spherical nucleus in an infinite G sphere under the prescribed external pressure p [Fig. 1(a)]. To obtain a simple analytical estimation we shall neglect several details, in particular finite strains. The variation of elastic moduli and thermal expansion will not be taken into account when defining the stress state and calculating the work integral in the PT criterion. Consequently, (10) can be used. The variation in elastic moduli and thermal expansion will be taken into account in an implicit way. In the particular case $\sigma_y = k = 0$ the PT pressure in (10) should coincide with the equilibrium pressure p_{eq}. We shall use (21) for p_{eq}, which includes the variation in elastic moduli and thermal expansion, and obtain

$$\theta_o = -\frac{a}{b}, \quad \rho\Delta s_o = \varepsilon_o b, \quad \Delta v = 0 \tag{22}$$

and

$$p = \frac{2}{3}\sigma_y\left(\frac{\sigma_y C}{\varepsilon_o} + \ln\frac{\varepsilon_o}{2\sigma_y C}\right) + \frac{k}{\varepsilon_o} + b(\theta - \theta_o). \tag{23}$$

Let us estimate the parameters in (23). The volumetric strain $\varepsilon_o = |1 - \rho_d/\rho_g = 0.5418$, where $\rho_d = 3.5 \times 10^3$ kg/m^3 and $\rho_g = 2.27 \times 10^3$ kg/m^3 are the mass densities of D and G in the unloaded state. The compression modulus of G at $p = 10$ GPa is equal to $K = 75$ GPa (Bundy, 1989). At $\nu_o = 0.3$ the constant

$$C = \frac{3(1-\nu_o)}{2E} = \frac{1-\nu_o}{2(1-2\nu_o)K} = 0.0117\,\mathrm{GPa}^{-1}. \tag{24}$$

For the yield stress we adopt the linear temperature dependence (Bell, 1973)

$$\sigma_y(\theta) = \sigma_y(0)\left(1 - \frac{\theta}{\theta_m}\right), \tag{25}$$

where $\theta_m = 4000$ K is the melting temperature of both G and D (G–D liquid triple point). We assume that at pressure $p = 10$ GPa, $\sigma_y(0) = 2$ GPa (Vereshchagin and Zubova, 1960). The result of the calculation of the PT pressure according (23) at $k = 0$ is shown in Fig. 2. The pressure increment due to mechanical work A_m/ε_o at $\theta = 0$ K is 3.34 GPa and at $\theta = 2000$ K is 2.11 GPa. If we assume that the difference between the experimentally defined PT pressure (approximately $p_{ex} = 11.26$ GPa at arbitrary temperature) and the pressure according to (23) at $k = 0$ is due to k, then the ratio k/A_m is maximum at $\theta = 0$ K and equal to 1.97; at $\theta = 2000$ K, $k/A_m = 1.386$; at $\theta = 3000$ K, $k/A_m = 0.957$. As these values are relatively small in comparison with $k/A_m = 9.445$ for steel, our assumption is plausible. It is interesting to note that the coefficient L in (1) varies from 3.35 to $\theta = 0$ K to 2.40 at $\theta = 3000$ K. This is a very narrow interval when we take into account the rather simplified character of our description.

Consequently there are two main reasons why the experimental PT pressure significantly exceeds the pressure calculated using the methods of chemical thermodynamics:

- the negative pressure variation in the course of the PT and corresponding mechanical work;
- the dissipation due to the PT.

Let us consider the appearance of the D nucleus in a liquid sphere which is located in a finite G sphere under the prescribed external pressure p [Fig. 1(b)]. As an initial condition assume that the pressure in the liquid and the prescribed pressure are the same. The liquid acts in three ways.

- First, the melted metal in the given case transforms a martensitic PT into a diffusive PT (Kurdyumov, 1980; Novikov *et al.*, 1987; Bundy, 1989), for which the dissipative threshold is zero.
- Second, the maximum possible pressure variation in the transforming particle in the liquid is $\Delta p = K_l(\upsilon_d - \upsilon_g)/\upsilon_l$, where υ_g, υ_d and υ_l are the volume of the transforming particle before and after PT and the volume of liquid, respectively. The volume of liquid is usually comparable with the volume of G sphere and the pressure variation in an infinitesimal D nucleus is negligible, because $\upsilon_l \gg (\upsilon_g - \upsilon_d)$.
- Third, let us consider the case where the volume of the transforming particle is comparable with the volume of the liquid drop. Due to the diffusion of liquid metal in G the effective yield stress of the graphite–metal mixture is very small. For a small drop we can apply (23) with

$$\varepsilon_o = \frac{\upsilon_g - \upsilon_d}{\upsilon_l} = \left(-1 + \frac{\rho_d}{\rho_g}\right)\frac{\upsilon_d}{\upsilon_l} = 0.5418\frac{\upsilon_d}{\upsilon_l}. \tag{26}$$

  For $\upsilon_d/\upsilon_l = 1/3$ and $\sigma_y = 0.2$ GPa, $p - p_{eq} = 0.440$ GPa.
  For $\upsilon_d/\upsilon_l = 1/6$ and $\sigma_y = 0.1$ GPa, $p - p_{eq} = 0.220$ GPa.
  For $\upsilon_d/\upsilon_l = 1/6$ and $\sigma_y = 0.01$ GPa, $p - p_{eq} = 0.037$ GPa.

  As diamond synthesis with liquid metals usually concerns $\theta = 1600 \div 2000$ K, i.e. at $p_{eq} = 5.25 \div 6.25$ GPa, then even the biggest deviation 0.440 GPa lies inside the experimental errors for high pressure–high temperature measurements.

Consequently there is no reason why the experimentally determined pressure needed for the appearance of a small D nucleus should exceed the pressure calculated using the methods of chemical thermodynamics. Thus the thermodynamical continuum theory developed allows us to explain both the fundamental experimental results mentioned above without any additional physical or chemical hypothesis.

If we want to model the process of metal melting in G, then we should introduce the volumetric transformation expansion in the metal and vary the elastic properties. At fixed elastic moduli the volumetric transformation expansion results in pressure growth in the liquid. Consequently the PT G–D can occur at the external pressure, which is less than the equilibrium p_{eq} pressure. The same will occur when the compression modulus of the chosen liquid is higher than the compression modulus of the G at zero transformation expansion. It is known that the pressure in the reaction cell increases due to the metal melting (Shul'zhenko *et al.*, 1977), i.e. the possibility of D synthesis under a pressure that is less than the equilibrium p_{eq} pressure can be real.

From this example we can derive three useful conclusions:

- —it is possible to use liquid or material with a small yield limit to decrease negative pressure variation in the course of the PT;
- —it is necessary to replace a martensitic PT by a diffusive PT in order to remove the dissipative threshold in the PT criterion;
- —PT conditions can be improved by the creation of a pressure (stress) concentration in the transformation zone, for instance by using another PT with corresponding transformation strain or material with higher elastic moduli.

3. ALLOWING FOR DISPLACEMENT DISCONTINUITIES: NONCOHERENCE AND FRACTURE

One of the mechanisms for getting more profitable stress variation in the transforming particle is related to the possibility of displacement discontinuities on the moving or fixed (at nucleation) interface. The jump of displacements tangential to the interface produces so-called noncoherence and is connected with the generation and sliding of dislocations on the interface with the Burgers vector tangential to the interface. The jump of the displacement component normal to the interface is a fracture.

3.1. *Noncoherence*

Earlier (Christian, 1965; Roitburd, 1972; Boguslavskiy, 1985), the possibility of noncoherent PT in elastic materials was estimated by comparing the energy of a coherent nucleus (displacements are continuous) and a noncoherent nucleus while taking into account the energy of dislocations. Now it is clear that the sliding along the interface is a dissipative process and comparison of energies is not sufficient. The dissipative concept in the theory of noncoherent PT was developed by Levitas (1992, 1995). We will present a simplified and modified version of this approach. For the points of noncoherent interface, the rate of dissipation due to sliding takes the form

$$\mathscr{D}_s = \boldsymbol{\tau} \cdot [\boldsymbol{v}_s] - \dot{\psi}_s([\mathbf{u}_s]) \geqslant 0, \tag{27}$$

where $[\mathbf{u}_s]$ is the displacement discontinuity, $\boldsymbol{v}_s = \dot{\mathbf{u}}_s$, $\boldsymbol{\tau}$ the shear stress and ψ_s is the energy of the displacement discontinuity (dislocations). After obvious transformations we obtain

$$\mathscr{D}_s = \left(\boldsymbol{\tau} - \frac{\partial \psi_s}{\partial [\mathbf{u}_s]}\right) \cdot [\boldsymbol{v}_s] = \mathbf{X}_s \cdot [\boldsymbol{v}_s] = \mathscr{D}_s([\boldsymbol{v}_s], [\mathbf{u}_s]), \tag{28}$$

where $\mathbf{X}_s = \boldsymbol{\tau} - \partial\psi_s/\partial[\mathbf{u}_s]$ is the dissipative force conjugated to $[\boldsymbol{v}_s]$. The dissipation function $\mathscr{D}_s([\boldsymbol{v}_s], [\mathbf{u}_s])$ should be determined experimentally; for time-independent martensitic transformations it is a homogeneous function of degree one in $[\boldsymbol{v}_s]$. Using the postulate of realizability (Levitas (1992, 1995) (or other postulates of irreversible thermodynamics or plasticity theory)) it is easy to obtain $\mathbf{X}_s = \partial\mathscr{D}_s/\partial[\boldsymbol{v}_s]$. For the isotropic case we get

$$\mathscr{D}_s = \tau_s|[\boldsymbol{v}_s]|, \quad \mathbf{X}_s = \tau_s \frac{[\boldsymbol{v}_s]}{|[\boldsymbol{v}_s]|}, \quad |\mathbf{X}_s| = \tau_s \quad \text{and} \quad [\boldsymbol{v}_s] = |[\boldsymbol{v}_s]| \frac{\mathbf{X}_s}{\tau_s}, \tag{29}$$

where τ_s is the dissipative threshold for the occurrence of sliding, at $|\mathbf{X}_s| < \tau_s$ sliding is impossible and the interface is coherent.

In the first approximation we assume that the processes of PT and sliding along the interface are thermodynamically independent, i.e. the driving force X in the PT criterion (1) (or in the general criterion in Part I) is independent of $[\boldsymbol{v}_s]$ and the driving force $\mathbf{X}_s$ in the sliding criterion (29) is independent of the rate of PT, e.g. of the interface velocity v_n (coupling between $[\boldsymbol{v}_s]$ and v_n is considered in papers by Levitas (1992, 1995)). Then these processes will interact through the stress field variation due to both of them.

The scheme of application of criteria (1) and $(29)_3$ is as follows. We model the appearance of a new nucleus in some volume by growth of the transformation strain (parameter ξ) and variation in material properties. If for a given ξ the sliding criterion is not met, then the interface is coherent. If for a given ξ the sliding criterion $(29)_3$ is satisfied, we admit the sliding at this point until a value where criterion $(29)_3$ is violated. After completing the PT we check with criterion (1) whether it is thermodynamically admissible. Consequently, growing transformation strain produces the stresses that are necessary for the appearance of noncoherence, and noncoherence changes the stress variation in the transforming particle.

As an illustration we consider a simple plane strain problem for a half-space. Suppose that, under the action of homogeneously distributed normal stress p over the length a, PT occurs in a triangle OEF (sides OE and OF are orthogonal); the rest of the half-space is rigid (Fig. 3).

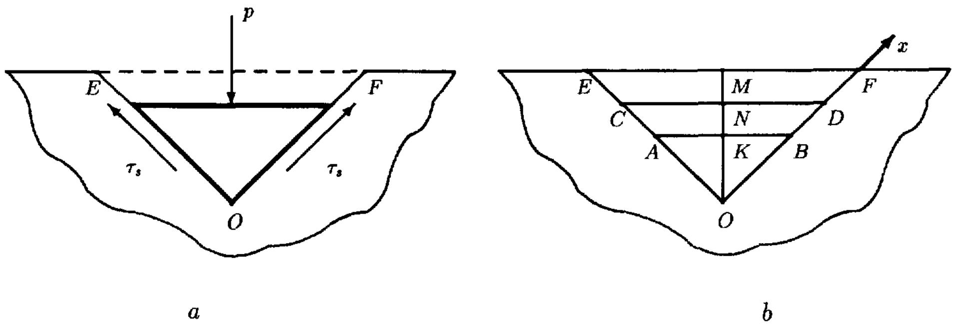

Fig. 3. Noncoherent PT in a half-space.

The same solution is valid in the case of homogeneously distributed normal stresses on the whole surface of the half-space. Such a situation can be realized both on the external and internal boundaries of a body, e.g. in the pores and cracks which contain liquid or gas.

The transformation strain $\boldsymbol{\varepsilon}^t = 0.5\varepsilon_0\mathbf{i}$, the plastic strain $\boldsymbol{\varepsilon}^p = 0$ in the triangle OEF, where $\varepsilon_0 = 1 - V_{n2}/V_{n1}$. Along the interfaces OE and OF, $[\mathbf{u}_s] \neq 0$, i.e. noncoherent PT occurs. Assume that the shear stress along the interfaces OE and OF is constant, $\tau = \tau_s \leqslant 0.5\sigma_y$, where σ_y is the yield limit of weaker material, i.e. the energy of dislocations is neglected. From the plastic limit equilibrium theory we obtain that at $p < (1+0.5\pi)\sigma_y$ the half-space is rigid (Hill, 1950). The nucleation condition (2) will be used with $V_n = V_{n1}$. In the given problem we can consider also a large ε_0, if we assume that the values $\Delta\psi^\theta$ and k are referred to the unit volume of phase 1.

In Fig. 3(b) three positions of the triangle are shown: initial *OEF*, final *OAB* and arbitrary intermediate *OCD*. Initial and finite geometric parameters have indices 1 and 2 ($EF = a_1$, $OF = b_1$, $OM = h_1$, $AB = a_2$, $OB = b_2$, $OK = h_2$), current parameters have no indices ($CD = a$, $OD = b$, $ON = h$). We will use in the calculation that

$$\frac{a}{h} = \frac{a_1}{h_1}, \quad a_1 = 2h_1, \quad V_{n1} = h_1^2, \quad V_{n2} = h_2^2, \quad \varepsilon_0 = 1 - \left(\frac{h_2}{h_1}\right)^2. \tag{30}$$

By taking into account the variation in geometry in the course of PT and (30) we obtain for the work of A_p of p

$$A_p = -\int_{h_1}^{h_2} pa\,\mathrm{d}h = -p\frac{a_1}{h_1}\int_{h_1}^{h_2} h\,\mathrm{d}h = -p(h_2^2 - h_1^2) = p\varepsilon_0 V_{n1} \quad (p > 0). \tag{31}$$

For each b, the power of the shear stresses τ_s along lines *OD* and *OC* is

$$\mathcal{D}_s = 2\tau_s \int_0^b v_s(x)\,\mathrm{d}x = 2\tau\int_0^b \frac{x}{b}\dot{b}\,\mathrm{d}x = \tau_s b\dot{b}, \tag{32}$$

where $v_s(x) = x/b\dot{b}$ is the velocity of relative sliding at point x (as the deformation of a triangle *OCD* is homogeneous, $v_s(0) = 0$ and $v_s(\mathrm{b}) = \dot{b}$). The total work A_s of the shear stresses

$$A_s = \int_{t_1}^{t_2} \mathcal{D}_s\,\mathrm{d}t = \tau_s\int_{b_1}^{b_2} b\,\mathrm{d}b = 0.5\tau_s(b_2^2 - b_1^2) = \tau_s(h_2^2 - h_1^2) = -\tau_s\varepsilon_0 V_{n1}. \tag{33}$$

As the left side of (2) is equal to $A_p + A_s$, then we have

$$p_{1\to 2} = \tau_s + \frac{\Delta\psi^\theta + k_{1\to 2}}{\varepsilon_0}. \tag{34}$$

Similar calculations give

$$p_{2\to 1} = -\tau_s + \frac{\Delta\psi^\theta - k_{2\to 1}}{\varepsilon_0}, \quad H = p_{1\to 2} - p_{2\to 1} = 2\tau_s + \frac{k_{1\to 2} + k_{2\to 1}}{\varepsilon_0}. \tag{35}$$

Consequently, at maximum possible $\tau_s = 0.5\sigma_y$ the expressions for $p_{1\to 2}$ and H for a noncoherent nucleus and (22) for $\sigma_n^{1\to 2}$ and H in the problem with the horizontal layer at $\tau = 0$ (see Part I) coincide and both variants are equiprobable. At $\tau_s < 0.5\,\sigma_y$ the noncoherent nucleation is more profitable (from the point of view of the postulate of realizability) than the nucleation in the horizontal layer.

Comparison of (44) from Part I for the nucleation in the inclined layer at $\gamma^t < \varepsilon_o$ and (34) shows that at small enough τ_s [$\tau_s < 0.5\sigma_{y2}(1-\gamma^t/\varepsilon_o)$] the noncoherent nucleation is more profitable than the nucleation in the inclined layer as well. Consequently the variation of τ_s is a way to control the PT pressure, geometry and type of nucleus.

3.2. *Fracture*

The jump of the component of displacement normal to the interface, or fracture, can be considered in a similar way to noncoherence. We assume that PT and fracture criteria are mutually independent, and that these processes are coupled through the stress fields only. If—in the course of growth of transformation strain (parameter ξ) and variation of material properties in the nucleus—some chosen fracture criterion is met at some point of the interface (or at other points), the crack should be introduced. Practically this results in the introduction of a new boundary with zero normal and shear stresses. After completing the PT we check with criterion (1) as to whether PT is in fact possible. Consequently, a growing transformation strain generates the stresses that are necessary for the fracture, and fracture changes the stress variation in the transforming particle. We should not take into account the variation of surface energy in the PT criterion, because it should be taken into account in the fracture criterion.

As an illustration we consider the problem of the appearance of a spherical nucleus in an infinite elastoplastic sphere under applied external pressure p (Section 2). As the simplest fracture criterion we assume that, if the tensile stress normal to the interface (the same as the pressure in the nucleus) reaches some critical value σ_c, the interface and consequently the nucleus becomes stress free.

Assume that the fracture occurs in the plastic region and (6) for $\tilde{p}_p$ is valid. From the condition $\tilde{p}_p = -\sigma_c$ we obtain the critical value of transformation strain

$$\varepsilon_{oc} = 2\sigma_y C \exp\left(\frac{1.5(p+\sigma_c)}{\sigma_y} - 1\right), \tag{36}$$

at which fracture occurs. At $\varepsilon_o > \varepsilon_{oc}$ pressure and mechanical work in the nucleus are zero. Consequently in (7), (8) and (10) the value ε_{oc} should be used instead of ε_o. If p is given, then equations (10) are linear equations relative to the temperature. When the temperature is prescribed, then equations (10) are nonlinear equations relative to p (as ε_{oc} is a nonlinear function of p).

Reduction in the strength of the interface σ_c significantly increases the work integral in (7) and improves the PT condition. In the ideal case $\sigma_c = 0$, the work integral in (7) is positive and reaches its maximum value.

The same effect can be reached by using some intermediate materials (layers) around the places of expected nucleation, e.g. brittle materials with small σ_c or without cohesion to parent phase or liquid. Note that the methods of control of the PT condition through the variation of interface tensile σ_c and shear τ_s strength are restricted by the possibility of obtaining only relatively small crystals, because they cannot grow. This can be important for producing superhard material powder (D, cubic boron nitride).

The numerical study of the interaction of PT, noncoherence and fracture is considered by Levitas *et al.* (1996). The averaging procedure for finite strains allowing for displacements discontinuity is treated by Levitas (1996c).

4. MODELLING OF THE TECHNOLOGICAL PROCESS OF DIAMOND SYNTHESIS

The industrial synthesis of D is a very complicated nonstationary and inhomogeneous process. One of the types of high pressure apparatus (HPA) for diamond synthesis is shown in Fig. 4 (Novikov *et al.*, 1991a). The symmetry of the HPA about the vertical axis OA and horizontal plane OB makes it possible for us to limit the study to one quarter of its axial section.

The reaction mixture consists of G and metal and after PT G–D of D as well. A container made of rock (pyrophillite, lithographic limestone) plays the role of a deformable gasket. The heater is a mixture of G and rock. A cemented carbide die is press-fitted in a block of steel rings. Two compound plates reduce axial stresses acting on a plate of a press.

Such a system is compressed by the press to a pressure in a reaction mixture of 4.5–

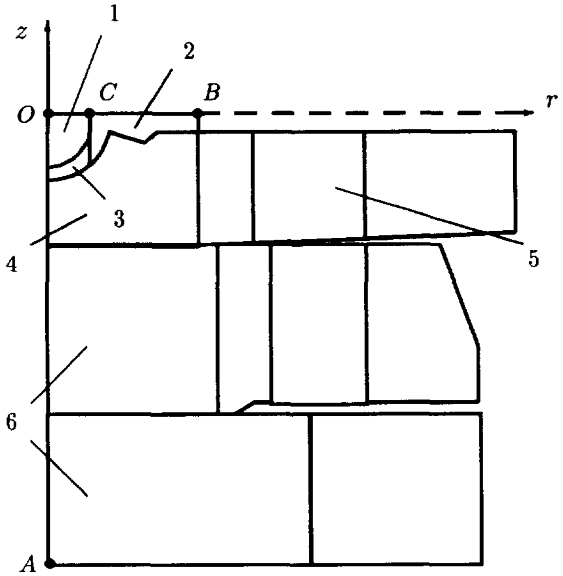

Fig. 4. High pressure apparatus for the diamond synthesis: 1—reaction mixture; 2—container; 3—heater; 4—die; 5—block of rings; 6—compound plates.

5.5 GPa. The reaction mixture is heated to the diamond synthesis temperature (1600–2000 K) by passing a low-voltage current through the mixture. Then the metal is melted and G is dissolved in a metal. If the pressure exceeds the equilibrium value (21) for the G–D system, then carbon is crystallized in the form of D.

It is known that good-quality D can be obtained near the equilibrium line (21) only (Kurdyumov, 1980; Novikov *et al.*, 1987). It follows from known experiments (Prikhna *et al.*, 1978) and our simulation (Novikov *et al.* 1988, 1990, 1991b; Levitas *et al.*, 1989; Idesman and Levitas, 1995) that the temperature and pressure are distributed extremely inhomogeneously. The question arises: how is it possible to obtain D of good quality in some experiments under such inhomogeneous conditions? To answer this question we will use the results of our numerical modelling of D synthesis (Novikov *et al.*, 1988, 1990, 1991b; Levitas *et al.*, 1989; Idesman and Levitas, 1995).

First of all a compression of the system by the press is modelled (Novikov *et al.*, 1990; Idesman and Levitas, 1995). Large elastoplastic deformation of container, reaction mixture and heater, pressure dependence of mechanical properties and contact sliding on the boundary between the die and container are taken into account. The theory of large elastoplastic deformation of materials under high pressure developed by Levitas (1987, 1996b) is used. Then electrical heating, stress redistribution, metal melting and PT G–D were studied.

The thermostress state of the reaction mixture in the HPA is changed during electric heating which results in a pressure increase. At the same time, PT G–D occurs starting from some instant of heating corresponding to attaining technological parameters for diamond synthesis.

This in turn affects the distribution of electric, temperature and stress fields in the HPA. Therefore, the interdependence occurs between the processes of electrical and heat conduction, thermoplasticity and PT, i.e. there are relations of electric potential field to those of temperature, pressure and D fraction; of temperature field to electric potential, pressure and D fraction distributions; of stress fields to those of temperature and D fraction and of D fraction field to pressure and temperature distributions in the reaction zone. Besides, there are physical and geometrical nonlinearities caused by the temperature dependence of thermophysical properties, by the pressure dependence of elastic and plastic properties and by the occurrence of large elastic and plastic strains.

A corresponding finite-element model has been developed to describe processes occurring in HPA during diamond synthesis with allowance for features enumerated.

The complete system of equations comprises equations of the plastic flow theory with allowance for finite strains, equations of electrical conduction, equation of nonstationary heat conduction, the kinetic equation for the rate of the D crystals growth, and equations for carbon phase equilibrium (21) and metal solvent melting (Novikov *et al.*, 1988, 1990, 1991b; Levitas *et al.*, 1989). The reaction zone is considered to be a mechanical mixture of G, metal solvent and D, the efficient properties of which are determined depending on the component's properties and mass fractions. PT is taken into account through the changes in properties, mass fraction of D and the compressive volumetric transformation strain. The rate of D mass fraction change in the region of its possible synthesis (when the metal is melted and D is stable) is

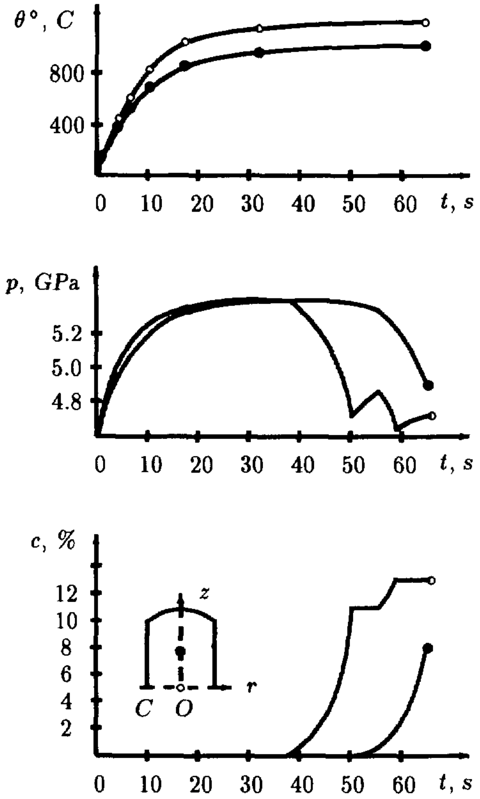

Fig. 5. Time dependence of temperature θ, pressure p and diamond volume fraction in two points of reaction mixture (Novikov *et al.*, 1991b).

determined by the topochemical Avraamy–Yerofeyev equation. The time dependence of temperature, pressure and volume fraction of D in two points of the reaction mixture is shown in Fig. 5. First D crystals appear in the centre of the mixture. Further, with D fraction increase and decrease in reaction mixture specific volume a monotone pressure drop is observed. At $t = 51$ s, D growth in the HPA centre ceases; this corresponds to the pressure drop below the equilibrium pressure for the G–D system.

At the same time diamond synthesis occurs in the neighborhood of the central point and pressure decreases there as well. As the force averaged over the line *OC* in the horizontal section of the HPA remains practically constant, the pressure at the point O increases.

The point O at the instant of time $t = 55$ s returns to the D stability region, D fraction growth is restarted, pressure drops again, and so on.

Consequently, an effect of pressure self-regulation is revealed which consists in the pressure oscillation near the G–D equilibrium line. D crystals grow near the equilibrium line due to this effect, which explains why it is possible to produce high-quality D under very inhomogeneous pressure and temperature fields.

5. POSSIBLE WAYS OF CONTROL OF PT CONDITIONS

Let us summarize our analysis of various useful examples of stress field variation in the transforming particle in the course of PT, giving possible ways of controlling PT by the purposeful control of stress–strain fields.

1. The trivial contribution of shear stresses to the driving force of PT connected with the work of shear stresses along the transformation shear strains.
2. According to the associated plastic flow rule, shear stresses and plastic shear strains (or plastic strain increments) are uniquely related, and they are in a monotone relation to each other, i.e. they produce equivalent contributions to the driving force of PT.
3. Effect of shear stresses on the yield conditions (problem of PT in an inclined layer):
   - Applied shear stresses contribute to the yield condition in a way equivalent to the decrease in the yield limit, and this is one of the mechanisms of an additional increase in the driving force of PT.
   - If a new phase has a yield stress $\sigma_{y2} \geqslant 2\sigma_{y1}$, shear stresses practically do not affect the PT condition.
   - Shear stresses can render the PT impossible, if due to the necessity of fulfilment of the yield condition for a parent phase a PT criterion is violated.
4. Possibility of an additional displacement to promote the PT for a significant volumetric transformation strain (problem of compression and shear of materials in Bridgman anvils). Ways of getting additional displacement are as follows:
   - reduction in contact friction due to the rotation of anvils or using some other methods;
   - reduction in yield stress under fixed applied load, e.g. due to heating;
   - use of the TRIP phenomenon during temperature cycling.

   These methods are especially effective for producing high-strength materials.
5. Creation of stress (pressure) concentration in the transformation zone:
   - by compression of a thin layer in Bridgman anvils;
   - by using another PT with corresponding transformation strain (e.g. metal melting at the PT G–D);
   - by using intermediate materials with higher elastic moduli (problem of G–D PT).
6. Decrease in the negative stress variation in the transforming region:
   - use of intermediate liquids or materials with a small yield limit;
   - reduction of interface shear strength τ_s to promote the noncoherence;
   - reduction of interface tensile strength σ_c or use of intermediate materials (layers) around the places of expected nucleation, e.g. brittle materials with small σ_c or without cohesion to the parent phase or liquid.

7. Reduction in the dissipative threshold k:
   - replacement of martensitic PT by diffusive PT;
   - reduction of the yield stress, e.g. by annealing or increasing the characteristic size (grain, subgrain, single crystal).
8. Search for and use of self-regulation phenomena for various systems.

6. CONCLUDING REMARKS

The results of the solution of problems of PT in elastic materials are in most cases easily understandable and interpretable due to the linearity of the equations. The non-trivial effects in plasticity are related to the necessity to meet the nonlinear yield condition in the parent and product phases and specific pressure redistribution. In particular, shear stress contributes to the driving force of PT even at zero transformation shear strain and in some cases pressure in the transforming region increases despite the volume decrease due to PT. The solutions obtained develop a nonlinear feeling of how PT proceeds in plastic materials and show much richer possibilities of control of PT.

Let us discuss qualitatively the effect of strain hardening on the PT condition based on the above solutions. Yield stresses of both parent and product (due to defects heredity) phases and consequently the dissipative threshold k increase with increasing plastic strain. Growth of k always makes the PT condition worse. As follows from the above equations (excluding in some cases (44) of Part I), in the case without external shear stresses the increase in yield stress reduces the driving force of PT. This explains the known experimental results (Bernshtein *et al.*, 1983; Hornbogen, 1984; Estrin, 1993) concerning the negative effect of preliminary plastic straining of austenite on PT.

In the problem of PT in the inclined layer at $0.5\sigma_{y2}\gamma^t > k\varepsilon_o$ in (42) of Part I the growth of the yield stress increases parameter A and if this increase exceeds the negative effect of growth of σ_{y2} in (41), the strain hardening improves the PT condition.

In the problem of the compression of materials in rotating Bridgman anvils the term $\bar{\tau}\gamma^t$ increases with increasing yield stress [see (47) in Part I of the paper (Levitas, 1997)]. At $\sigma_{y1} < \sigma_{y2}$ the increase in σ_{y2} which is larger than the growth in σ_{y1}, increases the pressure in the central part of the disk and improves the PT condition.

It is necessary to mention that at logarithmic strain of order 1, strain hardening is saturated. It was shown by Levitas (1987, 1996b) for more than 60 initially isotropic materials belonging to different classes (metals, rocks, oxides, compacted powder and powder mixtures) that for monotone (without unloading) and so-called quasi-monotone loading, beginning from a certain degree of deformation, materials are deformed as perfectly plastic, isotropic and strain-history independent. Due to the relation $(1)_2$ between k and σ_y, it is reasonable to assume that after some critical strain the value of k is also strain and strain-history independent. This hypothesis should be verified experimentally.

Based on the solutions obtained, the following experimental phenomena are described:

- preferential appearance of martensitic nuclei on slip surfaces;
- negative effect of preliminary plastic straining of austenite on PT;
- impossibility in some cases to transform the whole austenite into martensite without pressure (existence of a martensite finish temperature);
- negative effect of reduction of grain size or single crystal size on PT;
- linear dependence between pressure hysteresis and yield stress;
- decrease in PT pressure under applied shear stress or plastic strain and the possibility of PT at a pressure which is less than the thermodynamic equilibrium pressure;
- improvement in the condition of the PT in material compressed in Bridgman anvils due to the additional rotation of the anvil as well as the unique relation between the volume fraction of a new phase and the rotation angle of the anvil;
- possibility of obtaining new material phases under compression and shearing in Bridgman anvils, which are thermodynamically nonprofitable without rotation of the anvil;
- pressure self-multiplication effect due to PT in material compressed in Bridgman anvils;
- occurrence of direct solid–solid martensitic G–D PT at a pressure which is several times higher than the equilibrium pressure and the possibility of G–D PT at equilibrium pressure in the presence of some liquid metals;
- possibility of producing high-quality D under very inhomogeneous pressure and temperature fields.

All the above recommendations for the improvement of PT conditions are based on the simplest models and it is possible that more precise solutions may slightly or completely change some of them. These results are the formulation and first step to the solution of the problem of the search for possible ways to control PT in inelastic materials. It seems to us that systemization, experimental verification, further development and application of such recommendations can make a significant contribution to materials science and the synthesis of new materials.

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