Физика и техника высоких давлений 1997, том 7, №2

UDC 539.4:620.22

V.I. Levitas

DOES PLASTIC SHEAR AFFECT THE PHASE TRANSITIONS UNDER COMPRESSION OF MATERIALS IN BRIDGMAN ANVILS? NEW THEORETICAL STUDY

Institute of Structural and Computational Mechanics, University of Hannover,
Appelstraβe 9A, 30167 Hannover, Germany

Institute for Superhard Materials, Avtozavodskaya 2, 254074 Kiev, Ukraine

Paper has been received by 3 February 1997

Dedicated to my teacher
Professor N.V.Novikov
on the occasion
of his 65th birthday

A simple analytical description of phase transition (PT) under compression and shear of materials in Bridgman anvils is developed. It is found that an improvement of PT conditions due to a rotation of an anvil is attributed not to the plastic strain, but to a possibility of an additional axial displacement of an anvil, compensating a volume decrease because of PT. It is connected with a reduction of frictional shear stress in a radial direction due to the rotation of an anvil. The pressure self-multiplication effect and possibility of producing new hard materials due to rotation of an anvil are explained. Alternative ways of obtaining an additional axial displacement of an anvil are suggested.

After compression of materials in Bridgman anvils (Fig. 1), especially in diamond anvils, a very high pressure in the center can be reached. A number of PT can occur under such conditions. Additional rotation of an anvil and, consequently, plastic strain lead to significant reduction of PT pressure and to fundamentally new materials, which can not be produced without additional plastic strains. Volume fraction of the new phase is an increasing function of the rotation angle and, consequently, plastic shear strain. That is why plastic strain is considered as a factor producing new physical mechanisms of PT. It seems to us a little bit unrealistic. At the compression of materials in Bridgman nonrotating anvils, the mean value of plastic strain reaches 1000%, additional plastic shear strains near surfaces of anvils due to a contact friction exceed several thousand percent and have completely the same character as shear strain in rotating Bridgman anvils. Why no one of physical mechanisms of the effect of plastic strains on PT manifests itself at such high plastic shear strain, but appears at rotation of an anvil giving additional 10–100% plastic strain only?

In the paper a simple theory is developed, which gives a new look on the above phenomena.

Phase transition criterion

The criterion for PT nucleation in elastoplastic materials was derived [1–3] in the form

$$\int\int_{\varepsilon_1}^{\varepsilon_2} \sigma : \mathrm{d}\left(\varepsilon^e + \varepsilon^t\right) \mathrm{d}V - \int \Delta\psi \,\mathrm{d}V = \int k \,\mathrm{d}V, \tag{1}$$

where σ is the stress tensor, ε^e and ε^t are elastic and transformation strains, V is the volume of nucleus, ψ is the Helmholtz free energy per unit volume, k is the dissipation increment due to phase transition in a unit volume, related e.g. to the emission of acoustic waves and lattice friction, $\Delta\psi = \psi_2 - \psi_1$ (subscripts 1 and 2 denote the phase before and after PT). Formally Eq. (1) has the same form as for PT in elastic materials; plasticity affects implicitly a variation of σ in the course of PT and the k value. At equal elastic properties of phases we have [1–3]

$$\int\int_{\varepsilon_1^t}^{\varepsilon_2^t} \sigma : \mathrm{d}\varepsilon^t \,\mathrm{d}V - \int \Delta\psi^\theta \,\mathrm{d}V = \int k \,\mathrm{d}V, \tag{2}$$

where ψ^θ is the thermal part of the free energy, i.e. the elastic strains also disappear. Here we consider pure dilatational transformation strain $\varepsilon^t = 1/3\,\varepsilon_0^t I$, where I is the unit tensor, ε_0^t is the volumetric transformation strain. In this case, $\sigma{:}\mathrm{d}\varepsilon^t = p\,\mathrm{d}\varepsilon_0^t$, where p is the hydrostatic pressure. As the volumetric transformation strain and k are distributed homogeneously in the nucleus, Eq. (2) can be transformed to

$$\int_{\varepsilon_{01}^t}^{\varepsilon_{02}^t} \bar{p}\,\mathrm{d}\varepsilon_0^t - \Delta\psi^\theta = k, \quad \bar{p} = \frac{1}{V}\int p\,\mathrm{d}V, \tag{3}$$

where $\bar{p}$ is the averaged over the nucleus pressure. Eq. (3) is a final form of the phase transformation criterion which is used in the present paper.

Stress state of a thin cylindrical disk under compression and shear in anvils

We shall neglect the elastic deformations of anvils and deformed disk and use the well-known simplified equilibrium equation

$$\frac{\partial p}{\partial r} = -\frac{2\tau_r}{h}, \tag{4}$$

where r is the radial coordinate, h is the current thickness of the disk, τ_r is the radial component of the frictional shear stress τ at boundary S between anvils and a disk. Frictional shear stresses τ are directed opposite to the velocity v of relative sliding of a compressed material at boundary S. For a thin disk, the modulus τ reaches usually its possible maximum value equal to the half of yield limit σ_y. In the case without rotation of the anvil $\tau_r = 0.5\,\sigma_y$ and Eq. (4) yields

$$\frac{\partial p}{\partial r} = -\frac{\sigma_y}{h}; \quad p = \sigma_0 + \sigma_y\left(1 + \frac{R-r}{h}\right), \tag{5}$$

where boundary condition $p = \sigma_0 + \sigma_y$ at the external radius of anvil $r = R$ is taken into account, σ_0 is the pressure at $r = R$ due to external support of material being outside the working region of anvils $r > R$. Applied load is determined by integration of $p(r)$ over S

$$Q = \pi R^2 \left[\sigma_0 + \sigma_y \left(1 + \frac{R}{3h} \right) \right]. \tag{6}$$

Radial velocity u is defined from the incompressibility condition and condition $u = 0$ at $r = 0$ by the equation $u = -\dot{h}r/h$. During rotation of one of the anvils with an angular velocity ω expression for u is still valid, but the circumferential velocity $v = \omega r$ appears. In this case, velocity vector v and frictional shear stresses $\tau = 0.5\sigma_y v/|v|$ are inclined at an angle α to the radius with

$$\cos\alpha = \frac{u}{\sqrt{u^2 + v^2}} = \frac{1}{\sqrt{1 + \left(\omega h/\dot{h}\right)^2}} \tag{7}$$

and, consequently, $\tau_r = 0,5\ \sigma_y \cos\alpha$. Application of Eq. (4) with account for expression for τ_r leads to

$$p = \sigma_0 + \sigma_y \left(1 - \frac{R - r}{H} \right); \qquad Q = \pi R^2 \left[\sigma_0 + \sigma_y \left(1 + \frac{R}{3H} \right) \right]; \tag{8}$$

$$H = \frac{h}{\cos\alpha} = h\sqrt{1 + \left(\omega h/\dot{h}\right)^2}, \tag{9}$$

i.e. it is equivalent to the substitution of H for h. Let rotation occur at the fixed axial load Q. Then condition Q = const under the assumption σ_0 = const results in $H = \text{const} = h_0$, where h_0 is the thickness of the disk at the beginning of rotation, and in differential equation of reduction of thickness

$$d\varphi := \omega\, dt = \frac{dh}{h} \sqrt{\left(\frac{h_0}{h}\right)^2 - 1}. \tag{10}$$

Eq. (9) shows that at Q = const due to H = const, pressure distribution is independent of rotation, which corresponds to known experiments [4].

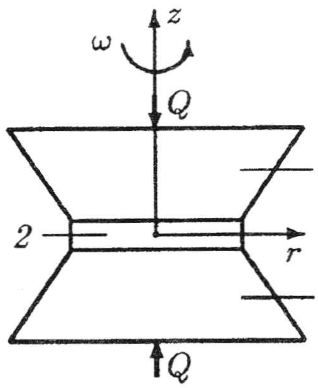
Consequently, rotation is equivalent to *reduction* of *friction* in the radial direction and results in a *decrease* of the *disk thickness* and this decrease is uniquely related to the rotation angle φ.

Let us consider PT in the central part of the disk and assume that transformation strain is a pure volumetric compression (Fig. 2). We adopt that the volume fraction of the new phase in transforming region A is c. In the case without rotation of the anvil one part of the disk material moves to the center of the anvil. A neutral circle EF with zero velocity of relative sliding can be easily found using a volume balance. Eq. (4) is valid, but shear stress in the region EF changes its sign and in the region A the yield stress σ_{y2} of a new material, which depends on c, should be used. We assume that the pressure is continuous across the interface. Results of an analytical solution are shown schematically in Fig. 2. It is important, that under a fixed axial force Q, pressure in the transforming region and the work integral in Eq. (3) decrease significantly, which makes PT condition worse. The higher σ_{y2}, the bigger pressure reduction in the transforming region.

Rotation, decreasing the thickness, reduces a negative pressure variation in the transforming particle. Optimal pressure variation (in the sense of the postulate of realizability [1,3,5]) will be, when infinitesimal radial flow from the disk center occurs. In this case shear stress does not change the sign, pressure monotonically grows with decreasing radius and volume decrease due to PT is completely compensated by the thickness reduction. The latter condition together with Eq. (10) at $\sigma_{y1} = \sigma_{y2}$ results in differential equation

$$d c \varepsilon_0 = \frac{d h}{h} = d \varphi \sqrt{\left(\frac{H}{h}\right)^2 - 1}; \quad c = \frac{1}{\varepsilon_0} \ln \frac{h}{h_0}, \tag{11}$$

which relates uniquely variation of volume fraction of new phase in transformed region and rotation angle, as is observed in experiments [6]. According to Eq. (4) if both phases have the same yield limit, pressure distribution after PT is the same as before PT (Fig. 2,*b*). If the new phase is weaker, pressure decreases in the center, if new phase is harder, pressure increases in the center. Consequently, despite the volume decrease due to PT, pressure increases due to the appearance of the harder phase and additional plastic flow, which agrees with experiments (the effect of pressure self-multiplication [4]).



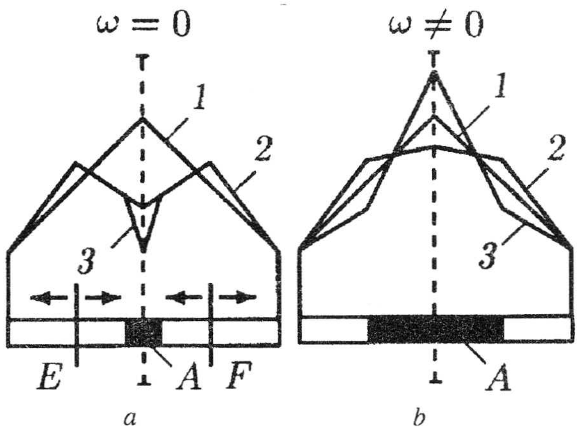


Fig. 1. Compression and shear of materials in Bridgman anvils: *1* – anvils; *2* – compressed material

Fig. 2. Pressure distribution: *a)* *1* – before PT, *2* – after PT at $\sigma_{y1} = \sigma_{y2}$, *3* – after PT at $\sigma_{y1} < \sigma_{y2}$; *b)* *1* – $\sigma_{y1} = \sigma_{y2}$, *2* – $\sigma_{y1} > \sigma_{y2}$, *3* – $\sigma_{y1} < \sigma_{y2}$

The above solution allows us easily to explain why rotation of an anvil gives us a way to obtain fundamentally new materials which cannot be produced under compression without rotation. If two materials can appear as a result of PT differing by the yield stress only, then the material with the smaller yield strength appears under compression without rotation (as pressure is higher at $\sigma_{y1} > \sigma_{y2}$, see Fig. 2,*a*), and the stronger phase will be obtained under compression with rotation (as pressure is higher at $\sigma_{y2} > \sigma_{y1}$, see Fig. 2,*b*). Consequently, the method based on the compression of materials with rotation of an anvil is especially important for the production of high-strength materials.

Note that explanation of pressure self–multiplication effect based on the increasing of elastic moduli after PT [4] is not correct, because it ignores the plasticity. Even at infinite moduli (as in our model), the pressure is limited by solution of the problem of plastic equilibrium, e.g. presented here. If $\sigma_{y1} > \sigma_{y2}$ or material flows to the center of the disk, the pressure in the new phase can not be increased irrespective of the increase in elastic moduli.

Let us summarize the results. Improvement of PT conditions due to rotation of the anvil is related to the possibility of additional displacement, compensating a volume decrease. It is connected with a decrease of friction stress in the radial direction. But when we understand that the reason is in additional displacement (and not in plastic straining), it is possible to find another ways to obtain additional displacement without rotation.

One possibility is to decrease the yield stress at constant external force, e.g. due to heating of the external part of the disk or the whole disk. Eq. (6) determines the variation of disk thickness, Eq. (11) defines the volume fraction of a new phase. As in the case with the rotating anvil, if a new phase is harder, pressure increases in the center of the disk. Such a situation is observed in experiments [7]: the increase in pressure caused by PT $B1 \rightarrow B2$ in KCl during heating from 300 to 600 K and initial pressure of 6 GPa at the center was 30%.

Another possibility may be based on the use of transformation – induced plasticity [8]. Let us consider a two-phase material consisting of inclusions in a plastic matrix. If under cyclic temperature variation, inclusions undergo the cyclic direct – reverse PT with large enough volumetric transformation strain, then the matrix will be deformed plastically even without external stresses. External stress produces plastic strain in the direction of its action, which is proportional to the value of applied stress and number of thermal cycles, i.e. is practically unlimited. If we introduce the transforming particles into the disk compressed in anvils, then it is possible to use the thermal cycles instead of rotation of the anvil to get additional displacement and to improve the PT condition in the center of the disk.

The pressure dependence of the yield stress and elastic strain will be taken into account elsewhere. The problem of compression of a rigid-plastic disk for pressure-sensitive materials is solved numerically in [9].

Concluding remarks

It follows from the solution of the above problems that the generally accepted statement concerning the improvement of the PT condition by large plastic shear is not always correct. Under uniformly distributed pressure and shear stress this is indeed the case [2,3,10], but in the case of rotating Bridgman anvils all impressive experimental results are described (at least qualitatively) without the appearance of plastic strain in any equation. Consequently, each experimental situation should be simulated carefully before any conclusion is made.

The phenomena enumerated in introduction take place not only for martensitic PT, but for various chemical reactions in polymers [11] and for oxide decomposition [12]. In these cases plastic shear accelerates the kinetics of reactions by several orders, making it practically "instantaneous" (like for martensitic PT), because volume fraction of product depends not on the time, but on the value of shear. This means, of course, the appearance of a new physical (or chemical) mechanisms. For martensitic PT this is not the case, because the "instantaneous" time-independent kinetics is typical of them without plastic strain as well. The existence of physical effect of plastic shear on martensitic PT can be proved only in the case of disagreement of experiment with the solution to the same problem, when all the material parameters and boundary conditions are determined independently.

Acknowledgements. The financial support of Volkswagen Foundation, as well as discussions with Prof. N.V.Novikov and E.Stein are gratefully acknowledged.

1. *V.I.Levitas,* Mech. Res. Commun. **22,** 87 (1995).
2. *V.I.Levitas,* Journal de Physique IV, Colloque C8, supplément au J. de Physique III, **5**, 173(1995).
3. *V.I.Levitas,* Journal de Physique IV, Colloque C2, supplément au J. de Physique III, **5,** 41 (1995).
4. *V.D.Blank, Yu.Ya. Boguslavski, et al.,* JEPT **87,** 922 (1984).
5. *V.I.Levitas,* Int. J. Eng. Sci. **33,** 921 (1995).
6. *M.M.Alexandrova, V.D.Blank, et al.,* Sov. Phys. Solid State, **30**, 577 (1988).
7. *V.D.Blank, Yu.Ya.Boguslavski, S.G.Buga,, E.S.Itskevich, Yu.S.Konyaev, and A.M.Shirokov,* High Pressure Science and Technology, Proc. XI AIRAPT Int. Conf., N.V.Novikov (ed.), 1989, Vol. 4, p. 64–66.
8. *K.A.Padmanabhan, and G.J.Dabies,* in: Superplasticity, Springer–Verlag, Berlin (1980).
9. *V.I.Levitas,* in: Large Deformation of Materials with Complex Rheological Properties at Normal and High Pressure, Nova Science Publishers, New York (1996).
10. *V.I.Levitas,* J. Mech. Phys. Solids, 1997 (in press).
11. *A.A.Zharov,* Uspekhi khimii **53,** 236 (1984).
12. *L.F.Vereschagin, E.V.Zubova, K.P.Burdina,, and G.L.Aparnikov,* Dokl. Akad. Nauk SSSR **196**, 81 (1971).