Strength of Materials, Vol. 28, No. 3, 1996

LARGE ELASTOPLASTIC STRAINS AND THE STRESSED STATE OF A DEFORMABLE GASKET IN HIGH PRESSURE EQUIPMENT WITH DIAMOND ANVILS

V. I. Levitas, S. B. Polotnyak, and A. V. Idesman UDC 539.893

A procedure is developed and realized in the form of a numerical modelling program for deformation of a gasket in diamond anvils taking account of the effect of high pressure and large elastoplastic strains for the material. The procedure is based on the finite element method with a stepwise iteration algorithm (the initial stress method). In the case of considerable distortion of the finite element network with large strains a procedure is used for redefining the network deformation. A package of programs for solving elastoplastic problems with large strains and high pressure developed at the Institute of Superhard Materials of the Ukrainian National Academy of Sciences is used in the calculations. Two materials are considered: hardened stainless steel T301 and pressed lithographic limestone (PLL). A degree of compression of a factor of eight is achieved for PLL (Odquist parameter $q \approx 5.5$, elastic volumetric strain (EVS) 0.7, pressure 24 GPa) and a factor of 5.8 for steel T301 ($q \approx 3$, EVS 0.7, pressure 50 GPa). The distribution of elastic and plastic zones during deformation and stress distribution over the anvil-gasket contact surface are obtained, and the stagewise nature of the deformation process is revealed.

In high-pressure equipment with diamond anvils (HPEDA) pressure is generated during compression of a deformable gasket between the anvils [1]. The gasket fulfils the role of deformable packing for the high-pressure zone and it is a force support for the anvil surfaces (due the ring of gasket material squeezed out around the edges of the ring) thus providing a distribution of stresses in the anvil and gasket surface so that they do not exceed permissible levels. Normally as a gasket material there is use [1] Niconel X750, hardened steel grade T301, Wapally, etc., in the form of a thin disk with an initial thickness of 150-300 μm.

A study of the behavior of gaskets used in HPEDA makes it possible to optimize conditions for generating ultrahigh quasistatic pressures and also to determine material properties with deformation by pressure in the megabar range. A number of tests have been undertaken for describing the compression of gaskets in diamond anvils [2-4]. The mathematical models obtained make it possible at the qualitative level to describe the deformation process. A common drawback of them is failure to consider features of the material deformation at high pressures involving the presence of high volumetric elastic and high plastic strains, and the dependence of gasket material yield strength on pressure.

The aim of the present work is a numerical study of the compression of deformable gaskets in diamond anvils taking account of the effect of high pressures and presence of large elastoplastic strains.

We consider two gasket materials: hardened stainless steel T301 (normally used for obtaining pressure of the megabar range) and pressed lithographic limestone (PLL). The latter is a standard material in synthesizing superhard materials and therefore its behavior at pressures in the megabar range is of considerable interest.

A typical feature of the problem in question is the fact that the gasket material experiences very marked plastic and considerable elastic volumetric strains (in compression the gasket thickness decreases by a factor of five to twenty depending on the magnitude of the pressures generated). We describe a model for the material. We shall assume that it is plastically incompressible since porosity which develops during plastic deformation at such high pressures should disappear. Volumetric elastic strains under high pressure are finite, but shear strains limited by the yield strength are small. Since gasket material strain is high and loading is uniform then a model for an ideally elastoplastic isotropic body is used [5]. A plasticity condition is used in the form of the Shleicher-Nadai criterion, and the rule for plastic flow in the deviator plane is associated with this criterion. In view of the fact that anvil and gasket geometry and also their loading conditions are close to axisymmetrical, the problem is solved in an axisymmetrical arrangement. In this case a closed set of equations (in the deformed current state) is written as follows [5].

V. N. Balkul' Institute of Superhard Materials, Ukrainian National Academy of Sciences, Kiev. Translated from Problemy Prochnosti, No. 3, pp. 78-87, March, 1996. Original article submitted July 27, 1992.

0039-2316/96/2803-0221$15.00

1. Equilibrium equations (with absence of volumetric forces)

$$\begin{cases} \frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0; \\ \frac{\partial \sigma_{rz}}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{\sigma_{rz}}{r} = 0. \end{cases} \tag{1}$$

2. Geometric relationships

$$d_{rr} = \frac{\partial \dot{U}_r}{\partial r}; \; d_{\theta\theta} = \frac{\dot{U}_r}{r}; \; d_{zz} = \frac{\partial \dot{U}_z}{\partial z}; \; d_{rz} = \frac{1}{2}\left(\frac{\partial \dot{U}_r}{\partial z} + \frac{\partial \dot{U}_z}{\partial r}\right); \tag{2}$$

$$W_{rz} = \frac{1}{2}\left(\frac{\partial \dot{U}_r}{\partial z} - \frac{\partial \dot{U}_z}{\partial r}\right); \; W_{rz} = - W_{rz}; \; W_{rr} = W_{zz} = W_{\theta\theta} = W_{r\theta} = W_{z\theta} = 0; \tag{3}$$

$$d_{ij} = \frac{1}{a^2} \tilde{B}^e_{ij} + d^p_{ij}; \; a^2 = \frac{2}{3}\left(B^e_{rr} + B^e_{zz} + B^e_{\theta\theta}\right) + 1; \tag{4}$$

$$\tilde{B}^e_{rr} = \dot{B}^e_{rr} - 2W_{rz}B^e_{rz}; \; \tilde{B}^e_{\theta\theta} = \dot{B}^e_{\theta\theta};$$

$$\tilde{B}^e_{zz} = \dot{B}^e_{zz} + 2W_{rz}B^e_{rz}; \; \tilde{B}^e_{rz} = \dot{B}^e_{rz} + W_{rz}(B^e_{rr} - B^e_{zz}).$$

(The nonlinearity of kinematic expansion (4) ($a \neq 1$) is caused by finite volumetric elastic strains).

3. Physical relationships in the elastic region $F = \sigma_i - \sigma_y(\sigma_0) < 0$

$$\sigma_{ij} = E_{ijmn}B^e_{nm} = \lambda B^e_{mm}\delta_{ij} + 2\mu B^e_{ij}, \tag{5}$$

and in the elastoplastic region $F = 0$

$$\tilde{\sigma}^e_{ij} = \left(E_{ijmn} - \frac{1}{N} E_{ijpq}S_{pq}\frac{\partial F}{\partial \sigma_{kl}} E_{lkmn}\right)a^2 d_{mn};$$

$$N = \frac{\partial F}{\partial \sigma_{ij}} E_{ijmn}S_{nm}; \; \tilde{\sigma}_{ij} = \dot{\sigma}_{ij} + \sigma_{ik}W_{kj} - W_{ik}\sigma_{kj}, \tag{6}$$

where indices i, j, k, l, m, n, p, q take the values r, θ, z (tensor components with pairs of indices rθ and θz equal zero and they should be excluded from consideration); σ_{ij} is true stress tensor (in the axisymmetrical case it contains four components: radial σ_{rr}, axial σ_{zz}, tangential $\sigma_{\theta\theta}$, and shear τ_{rz} stresses); d_{ij} is strain rate tensor; $d_{ij}{}^p$ is plastic strain rate tensor; W_{ij} is rotation tensor; $B_{ij}{}^e$ is Figner elastic strain tensor and it is assumed that the deviator components $Э^e_{ij} = B^e_{ij} - \frac{1}{3} B^e_{mm}\delta_{ij} << 1$; λ, μ are Lamé constants; $F = 0$ is the plasticity surface; $\sigma_i = \left(\frac{3}{2} S_{ij} \cdot S_{ji}\right)^{1/2}$ is stress intensity; $\sigma_y(\sigma_0) = K(1 + \rho\sigma_0)$ is yield strength; $\sigma_0 = {}^1/_3\sigma_{mm}$ is pressure; K, ρ are material constants; $S_{ij} = \sigma_{ij} - {}^1/_3\sigma_{mm}\delta ij$ is stress deviator; $\tilde{B}_{ij}{}^e$, $\tilde{\sigma}_{ij}$ is the Yauman derivative of tensors $B_{ij}{}^e$, σ_{ij} respectively; E_{ijkl} is elastic constant tensor; δ_{ij} is Kronecher symbol. We note that in the absence of plastic strains relationship (6) is written in the form

$$\tilde{\sigma}_{ij} = a^2 E_{lkmn} d_{mn}. \tag{7}$$

4. Standard boundary conditions in displacements or stresses.

In order to solve set of Eqs. (1)-(7) a finite element procedure is developed with a stepwise iteration algorithm [6] (the finite stress method). We note its features. A change-over from a differential to a variation arrangement is based on writing equilibrium Eqs. (1) in variational form using the principle of possible displacements (virtual work). A variable reference configuration is used agreeing with the strained configuration at the end of the preceding step (similar to a modified Lagraingian approach [7]). In the case of considerable distortions of the finite element network with large

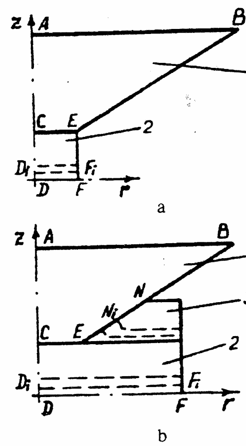

Fig. 1. Calculation scheme for determining the initial stressed state of a deformable gasket in high-pressure equipment with diamond anvils: a) pressed lithographic limestone; b) hardened steel T301 (1 is the diamond anvil; 2 is the deformable gasket; 3 is the region filled by the gasket material during compression).

strains a procedure is used for redefining the deformed network. In essence it involves the fact that a new finite element network is constructed (without distorted finite elements) whose boundaries coincide with the deformed contour of the previous network. Then by means of nodal values of some parameter (stress or displacements components) and iteration functions within an element for a deformed network nodal values are determined for this parameter in the newly constructed network from values of the coordinates of new nodes. With this procedure some distortion of the redefined parameter is possible if the new network contains few finite elements or the new interpolated functions are of a lower order. The magnitude of the error may be estimated for example by determining the difference of values of the parameter in question at a series of internal points of the region calculated for the deformed of new finite element network.

The test region is separated into triangular axisymmetrical linear finite elements (from 1500 to 2000 elements depending on the step in loading). A package of programs used in the calculation for solving elastoplastic problems with large strains [8] is realized in a ES series computer and a PC. It should be noted that with the aim of evaluating the accuracy of the results obtained for some loading steps the problem was solved in a finer finite element network (about 3400 elements). Here the difference in stresses did not exceed 4%.

The calculation scheme for solving the problem is presented in Fig. 1. The following boundary conditions are assumed: over surface AB there are no displacements in the direction of axis z ($u_z = 0$) and there are no shear stresses ($\tau_{rz} = 0$); over AD there are no displacements in the direction of axis r ($u_r = 0$) and $\tau_{rz} = 0$; over DF displacements are prescribed in the vertical direction: $u_z \neq 0$ and $\tau_{rz} = 0$; zero normal σ_n and tangential τ_n stresses are prescribed over the free surfaces. Over CE and EN contact conditions for the anvil 1 and gasket 2 are prescribed. Over CE the condition of absolute adhesion is prescribed (as shown in [4]), and the value of the friction coefficient between the anvil and the gasket, traditionally considered important for operation of a system with Bridgeman anvils, has a weak effect on the SSS if it is not too small. We describe conditions over EN. Here initially there are no contact conditions ($\sigma_n = \tau_n = 0$). With compression the gasket material deforms plastically and fills region 3 (Fig. 1b). The broken lines in Fig. 1 show the contour of the gasket at different stages of compression. With a change-over to a new finite element network conditions over EN change: over section EN_i contact conditions are prescribed for the anvil and gasket (similar to those prescribed for CE), but over N_iN the previous conditions remain ($\sigma_n = \tau_n = 0$).

In the calculations constants are also used for the materials in question: for diamond [9] Young's modulus E = 1070 GPa, Poisson's ratio $\nu = 0.07$; for steel T301, E = 260 GPa, $\nu = 0.2525$ [10], yield strength $\sigma_y = 1.6 + 0.002\sigma_0$ GPa; for PLL [5] E = 30 GPa, $\nu = 0.3$, $\sigma_y = 0.244 + 0.293\sigma_0$ GPa; for region 3 (Fig. 1) E = 0.01 GPa, $\nu = 0.2$.

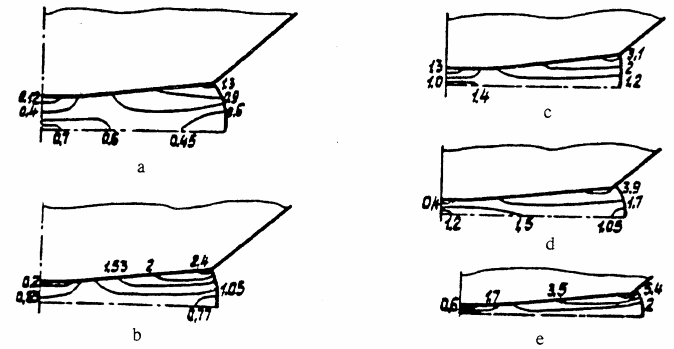

Fig. 2. Isolines for Odquist parameter q in a gasket made of PLL with compression by a factor of 1.7 (a), 2.6 (b), 3.57 (c), 5.0 (d) and 8.0 (e) in diamond anvils.

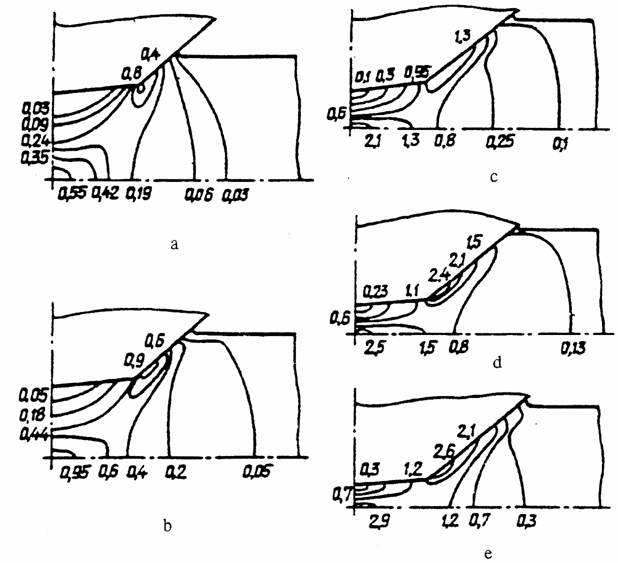

Fig. 3. Isolines for Odquist parameter q in a gasket made of hardened stainless steel T301 with compression by a factor of 1.36 (a), 1.63 (b), 2.8 (c), 3.8 (d), and 5.8 (e) in diamond anvils.

Modelling of the compression of a disk was carried out stepwise and in each step small vertical displacements u_z over surface DF were prescribed. As the shape of elements is distorted with large strains a change-over is accomplished to a new finite element network. The problem was resolved in an ES 10-45 computer. The time for considering one loading step was 10-60 min depending on the degree of gasket compression. Given in Figs. 2-4 are some data obtained for gaskets made of hardened stainless steel T301 and PLL in different stages of compression.

As a result of analyzing the distribution of elastic and plastic zones with deformation a stagewise compression was revealed for the gaskets:

in the initial stage the region of plastic strains in the gasket spreads from the periphery towards the center of the disk. The anvils draw together with formation of overlaps providing a force support of their surfaces. The maximum radius σ_{rr} and axial σ_{zz} stresses are found in the periphery of the operating surface of the diamond anvils;

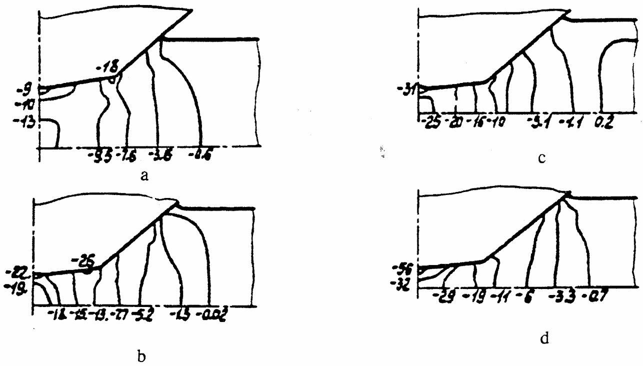

Fig. 4. Isolines for axial σ_{zz} stresses in a gasket made of hardened stainless steel T301 with compression by a factor of 1.63 (a), 2.8 (b), 3.8 (c), and 5.8 (d) in diamond anvils.

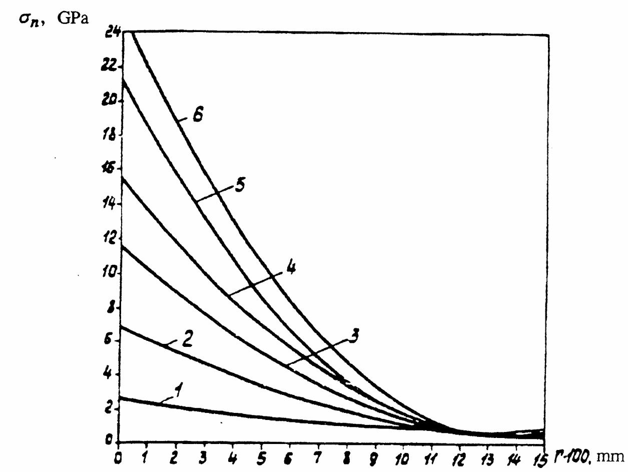

Fig. 5. Distribution of normal stresses σ_n over the contact surface for a diamond anvil-PLL gasket with compression by a factor of 1.17 (1), 2.6 (2), 3.57 (3), 5. (4), 6.14 (5), and 8.0 (6).

with further compression the plastic strain region embraces all of the gasket with the exception of a small zone under the anvil close to the axis of symmetry. Here there is a marked reduction in the dimensions of the elastic zone. As before maximum stresses occur at the periphery of the working surface of the diamond anvils;

a gradual increase in load leads to disappearance of the elastic zone and causes intense plastic flow of the gasket material. Here the region of maximum plastic strains is located at the periphery of the operating surface of the anvil.

With subsequent deformation the region of maximum plastic strains increases in size and gradually shifts towards the center of the operating surface of the anvils. Here the zone of greatest axial σ_{zz} and σ_{rr} stresses shifts from the periphery of the operating surface towards the center and with compression by a factor of 1.12 for PLL and 3.5 for steel T301 it reaches the center. Further compression leads to an increase in the level of plastic strains at the periphery of the operating surface and a rapid increase in axial σ_{zz} and radial σ_{rr} stresses at the center of it. The radial distribution of normal σ_n stresses over the anvil-gasket contact surface during compression for gaskets made of PLL and hardened steel T301 is illustrated in Figs. 5 and 6.

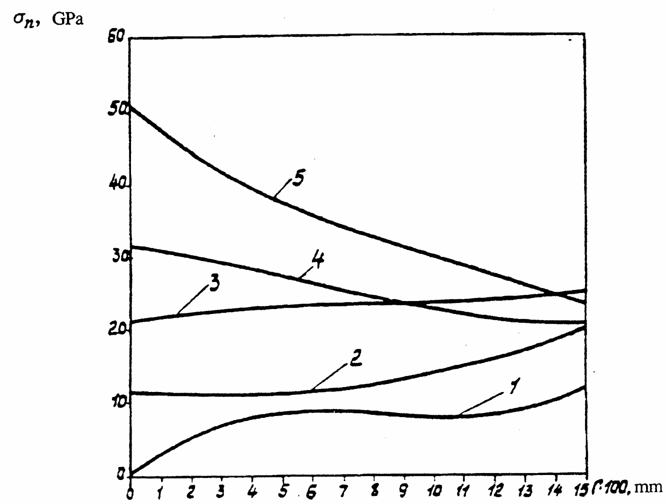

Fig. 6. Distribution of normal stresses σ_n over the contact surface of a diamond anvil-steel T301 gasket with compression by a factor of 1.36 (1), 1.8 (2), 2.8 (3), 3.78 (4), and 5.8 (5).

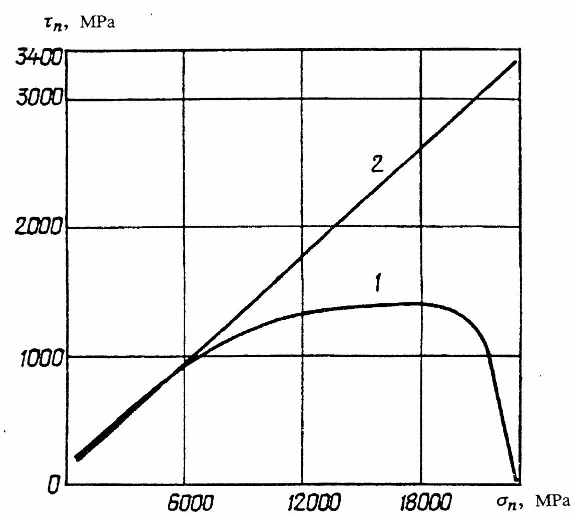

Fig. 7. Relationship $\tau_n = f(\sigma_n)$ for the contact surface of a diamond anvil-PLL gasket obtained by the FEM (compression by a factor of eight) (1) and the SLM [7] (2).

Given in Fig. 7 is the relationship $\tau_n = f(\sigma_n)$ for points of the contact surface of a PLL gasket compressed by a factor of eight (curve 1). Previously [5] a similar relationship was obtained $\tau_n = f(\sigma_n)$ using the sliding line method (SLM) on condition that for the contact surface the Coulomb plasticity condition is fulfilled, i.e. friction is the maximum possible and sliding occurs almost over the whole contact surface (curve 2 in Fig. 7). In order to solve the FEM problem with a condition of absolute adhesion it is found that in part of the contact surface (with $\sigma_n < 6$ GPa or $r > 0.07$ mm) conditions of maximum contact friction are fulfilled (Fig. 6). At the same time in the remaining part of the friction surface the maximum is not reached and the condition of absolute adhesion is correct there. Thus, the condition adopted for absolute adhesion over the contact surface leads to a correct result: presence of an adhesion zone (in which $\tau_n < \mu\sigma_n$, where μ is friction coefficient) and a zone with maximum friction. Large shear strains in the second zone model sliding in the thin contact layer.

It should be noted that comparison of the results obtained by us and the FEM with experimental data obtained in the Donets Physicotechnical Institute of the Ukrainian National Academy of Sciences with experimental studies of compression for metal gaskets in diamond anvils [3] confirm the reliability of the first results.

Thus, as a result of numerical modelling of the compression process for gaskets in diamond anvils a degree of compression by a factor of eight is achieved for PLL (Odquits parameter $q \approx 5.5$, magnitude of volumetric elastic strains $\varepsilon_0 \approx 0.7$, generated pressure ~24 GPa) and by a factor of 5.8 for steel T301 ($q \approx 3$, $\varepsilon_0 \approx 0.7$, pressure ~50 GPa); the distributions of elastic and plastic zones with deformation, distributions of stresses over the anvil-gasket contact surface are obtained, and the stagewise nature of the gasket deformation process is revealed. The results obtained were used in optimizing the construction of diamond anvils for high-pressure equipment [11].

LITERATURE CITED

1. A. Jayaraman, "Ultrahigh pressure," Rev. Sci. Instrum., **57**, No. 6, 1013-1031 (1986).
2. V. V. Kechin and E. N. Yakovlev, "Multiplication of pressure in high-pressure equipment of the anvil type," Fiz. Tekh. Vysokykh Davlenii, No. 23, 74-78 (1986).
3. A. V. Kurdyumov, V. P. Degtyareva, E. G. Ponyatovskii, et al., Effect of High Pressures on a Substance: in two vol., Vol. 1, Effect of Pressure on the Structure and Properties of a Substance (A. N. Pilyankevich, editor) [in Russian], Naukova Dumka, Kiev (1987).
4. D. J. Dunstan, "Theory of the gasket in diamond anvil high-pressure cell," Rev. Sci. Instrum., **60**, No. 12, 3789-3795 (1989).
5. V. I. Levitas, High Elastoplastic Strains for Materials at High Pressure [in Russian], Naukova Dumka, Kiev (1987).
6. V. I. Levitas and A. V. Idesman, "Features of solving thermoelastoplastic problems by the finite element method," Probl. Prochn., No. 10, 60-66 (1986).
7. M. S. Gadala, M. A. Dokainish, and G. A. Orovas, "Formulation of methods of geometric and material nonlinearity problems," Int. J. Numer. Meths. Eng., No. 20, 887-914 (1984).
8. N. V. Novikov, V. I. Levitas, and A. V. Idesman, "Theoretical description of thermomechanical effects in high pressure apparatus," High Pressure Research, **5**, 868-870 (1990).
9. J. E. Field (editor), The Properties of Diamond, Academic Press, London–New York–San Fransisco (1979).
10. W. C. Moss and K. A. Goettel, "Finite element design of diamond anvils," Appl. Phys. Lett., **50**, No. 1, 25-27 (1987).
11. N. V. Novikov and S. B. Polotnyak, "The numerical modelling of the stress-strained state of diamond anvil cell components," High Pressure Research, **5**, 865-867 (1990).