New model of plastic deformation of disordered systems

1993 J. Phys.: Condens. Matter 5 1633

(http://iopscience.iop.org/0953-8984/5/11/004)

J. Phys.: Condens. Matter 5 (1993) 1633–1642. Printed in the UK

New model of plastic deformation of disordered systems

O V Gendelman and L I Manevitch
Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia

Received 16 December 1991, in final form 9 November 1992

Abstract. The model of plastic phenomena in glasses is developed. Structural defects connected with the molecular states with a double-well potential are introduced. On the basis of this concept it turns out to be possible to explain the characteristic features of the deformation process. The values of the limit of proportionality, yielding limit and angle of propagation of shear bands are estimated for a two-dimensional glass. The results obtained are compared with the experimental data available and considerable agreement is observed.

1. Introduction

It is well known that the theoretical description of the plastic deformation of crystals deals with the concept of structural defects. It is possible to define the 'ground state of equilibrium' of a crystal as associated with an ideally ordered lattice. The other possible states of equilibrium are connected with the various local violations of this order and may be identified with the structural defects, e.g. dislocations, vacancies and disclinations. To investigate the behaviour of dislocational loops (in the three-dimensional (3D) case) under an external load we obtain quite a reliable model of plastic phenomena in crystals [1].

Glasses can also demonstrate plastic behaviour. On the macroscopic level the characteristic features of plasticity in glasses are quite similar to those in crystals. In particular, it is possible to observe the formation of shear bands and plastic flow of glass under a constant external load. However, it is difficult to define structural defects in a disordered structure; the random network of chemical bonds or the random packing of spheres (which are the common molecular models for glasses) both may possess many metastable states of equilibrium, which is very far from an ordered crystalline structure. There is no opportunity to distinguish one of these metastable states as a 'ground state' without defects. So, we should consider all possible structures of glasses as containing defects. Attempts to construct the appropriate theory on the basis of the generalization of the dislocation concept for glasses [2] were not successful.

The theory of topological defects in random networks was proposed by Rivier and Duffy [3, 4]. The defect structures which they considered are in fact odd-number ring chains which either end on the surface of the glass or form a closed loop. This approach is very powerful and useful for different problems concerning the behaviour of glasses but has not yet been applied for the description of plastic phenomena.

Nevertheless as a result of some computer and physical experiments it was established that the concept of structural defects may be useful to explain plastic

0953-8984/93/111633+10$07.50

phenomena in glasses. In the experiments of Argon and Kuo [5] the behaviour of the bubble model of a random-packed structure under a shear load was investigated. It was noticed that shear deformation was localized in 'small rings' of bubbles and proceeded without a considerable change in the free volume in these rings. Another experiment [6] was undertaken to study the behaviour of a plane system of ellipses interacting with each other only at the points of mechanical contact with forces of normal reaction and tangential friction. It was found that the plastic flow in such a system was accompanied by the formation of shear bands which were in fact lines of particles having an abnormally small number of contacts with their neighbours. The regions of local deformation in [5] and the regions with a small number of contacts in [6] may be regarded as similar to defects in a disordered system.

Other evidence that structural defects are important for the description of properties of glasses is provided by various experimental and theoretical explorations of anomalous low-temperature properties, such as heat capacity and heat conductivity [7, 8]. The existing phenomenological models introduce the concept of defects present in glasses, referred to as 'softons' [7] or 'states with double-well potential (SDWPs)'. The local motions connected with these defects and the scattering of long-wave phonons on these defects are responsible for the anomalies observed.

The main idea of the present paper is that the structural defects discovered by simulation and introduced into phenomenological theories of low-temperature properties are the same and are responsible for both the thermal and the mechanical properties of glasses. From the viewpoint of microstructure these defects, in our opinion, may be associated with disclination loops of minimal possible size. Large loops are regarded as 'diluted' in the elastic continuum and affect the average elastic properties only. They can hardly take part in plastic events because of their large size and the huge energy needed to create such a defect in material.

In the present paper for simplicity we deal with the two-dimensional (2D) model of glass. The model of defects in this case is constructed in section 2. The process of plastic deformation is considered in section 3. Then the results obtained are discussed in connection with the experimental data. Some other possibilities of the theory developed are also demonstrated.

2. Theory of a single defect

In the one-dimensional case the system with a double-well potential (DWP) may be obtained for the system given in figure 1. The interaction of particles is described by the usual Lennard–Jones potential:

$$U(r) = V[(\sigma/r)^{12} - (\sigma/r)^{6}]. \tag{2.1}$$

It is simple to demonstrate that for

$$r_0 > \sigma(26/7)^{1/6} \tag{2.2}$$

we obtain that atom 2 is in the DWP.

In order to develop the molecular model of structural defects in a 2D glass we consider the system presented in figure 2. Atom 2 is replaced in direction 1–2 to create a DWP for atom 1. In another direction the potential for atom 1 remains of

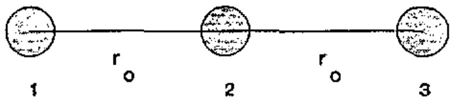

Figure 1.

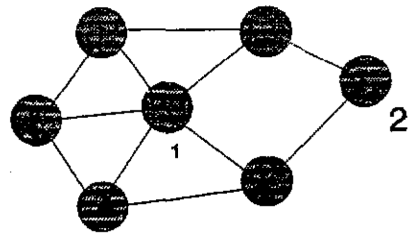

Figure 2.

a single-well nature. The presence of atoms in the first sphere of coordination may result in asymmetry of the DWP. If we regard the third sphere of coordination as fixed, it is possible to obtain a stable configuration. Such a model of a defect with a DWP is applicable for describing the thermal properties of glasses. The low coordination number of atom 1 corresponds to the small number of contacts in [6]. To describe the mechanical properties, however, we need the quantitative description of a defect.

The displacements of atoms in the second sphere of coordination are small enough to use the theory of elasticity to describe the long-range field of displacements, caused by the defect. In order to define the rate of decrease in displacements at long distances from the core of the defect, we recall that the appearance of the defect introduced leads to local changes in the structure of the disordered system only (the appearance of a dislocation in the crystal, on the contrary, needs an additional atomic half-plane and so cannot be reduced to the local changes in structure). So, the effect of the changed fragment on the rest of the structure (which is regarded as the elastic continuum) in the first order of magnitude is reduced to the action of an equilibrium pair of forces (dipole component). The action of the force pair leads in the 2D case to a decrease in the rate R^{-1} (for the displacement field) [18].

Also, in the 3D case the structure, analogous to that in figure 2, may be described as a disclination loop of the minimal size possible [3] and such a system is also an SDWP [3]. According to [4], the strain field of the disclination line in a glass decreases as R^{-1} owing to the effect of screening. So the displacement field of a loop decreases as R^{-2}. Similarly, in the 2D case we may also assume that the field of the defect introduced decreases as R^{-1}. Here we suppose that the concentration of defects considered is sufficiently small that it is possible to disregard the quadrupole and higher-order components, which, of course, implies the other decreasing rates.

Now it is possible to calculate the elastic field of the defect.

The equilibrium equations in polar components are written

$$\begin{aligned} &\partial\sigma_r/\partial r + \tfrac{1}{2}\tau_{r\vartheta}/\partial\vartheta + (\sigma_r - \sigma_\vartheta)/r = 0 \\ &(1/r)(\partial\sigma_\vartheta/\partial\vartheta) + \partial\tau_{r\vartheta}/\partial r + 2\tau_{r\vartheta}/r = 0. \end{aligned} \tag{2.3}$$

From Hooke's law,

$$\begin{aligned} \sigma_r &= \lambda(\epsilon_r + \epsilon_\vartheta) + 2\mu\epsilon_r \\ \sigma_\vartheta &= \lambda(\epsilon_r + \epsilon_\vartheta) + 2\mu\epsilon_\vartheta \\ \tau_{r\vartheta} &= \mu\gamma_{r\vartheta} \end{aligned} \tag{2.4}$$

where λ and μ are the Lamé constants; the expressions for the components of strain tensor are

$$\epsilon_r = \partial u_r/\partial r \qquad \epsilon_\vartheta = (1/r)(\partial u_\vartheta/\partial\vartheta)$$
$$\gamma_{r\vartheta} = \partial u_\vartheta/\partial r - u_\vartheta/r + (1/r)(\partial u_r/\partial\vartheta) \tag{2.5}$$

with $\boldsymbol{u} = (u_r, u_\vartheta)$ being the vector of the displacement, and assuming that

$$\boldsymbol{u} = (1/r)\boldsymbol{V}(\vartheta). \tag{2.6}$$

Thus we finally obtain

$$sV_r'' - 2V_\vartheta' = 0$$
$$V_\vartheta'' + 2sV_r' = 0 \qquad s = \mu/(\lambda + 2\mu). \tag{2.7}$$

The symmetry conditions for (r, ϑ) may be obtained if one recalls that the defect introduced is anisotropic. Choosing for direction 1–2 the condition $\vartheta = 0$, we have

$$V_r(\vartheta) = V_r(-\vartheta). \tag{2.8}$$

Solving the system (2.7)–(2.8), we obtain

$$\begin{pmatrix} V_r \\ V_\vartheta \end{pmatrix} = A \begin{pmatrix} \cos(2\vartheta) + c \\ -s\sin(2\vartheta) \end{pmatrix}. \tag{2.9}$$

Equation (2.9) becomes invalid at distances $r < a_0$, where a_0 is the core size of the defect, which is of the order of the interatomic distance. We may estimate the discontinuities of the displacement field: in the direction $\vartheta = 0$,

$$[u_r] \simeq |A(1 + c)|^{1/2} \tag{2.10a}$$

and in the direction $\vartheta = \pi/2$,

$$[u_r] \simeq -|A(1 - c)|^{1/2}. \tag{2.10b}$$

From (2.2) we have $[u] \simeq 0.3a_0$. So, for A, we have the estimate

$$A/a_0^2 \simeq 0.1/(1 + c). \tag{2.10c}$$

Now it is possible to calculate the elastic energy of a single defect. For the strain tensor we have

$$\epsilon_r = -[A\cos(2\vartheta)]/r^2$$
$$\epsilon_\vartheta = [A(1 - 2s)\cos(2\vartheta)]/r^2 \tag{2.11}$$
$$\gamma_{r\vartheta} = [2A(s - 1)\sin(2\vartheta)]/r^2$$

and for the stress tensor σ_{ij} we obtain

$$\sigma_r = A[c\lambda - 2\cos(2\vartheta)(s\lambda + \mu)]/r^2$$
$$\sigma_\vartheta = Ac(\lambda + 2\mu)/r^2 \tag{2.12}$$
$$\tau_{r\vartheta} = \mu\gamma_{r\vartheta}.$$

The energy density in polar components is expressed by the Clapeyron formula

$$w = \tfrac{1}{2}(\sigma_r \epsilon_r + \sigma_\vartheta \epsilon_\vartheta + \tau_{r\vartheta}\gamma_{r\vartheta}). \tag{2.13}$$

Finally we have for the energy of the defect

$$W = \pi A^2[c^2(\lambda + 2\mu) + 2\mu(1-s)(2-s)]/2a_0^2 + E_c \tag{2.14}$$

where the energy E_c of the core may be roughly estimated as $\mu A^2/a_0^2$.

The total energy of a glass with structural defects may be expressed as

$$\mathbb{W} = W_{ex} + W_{def} + W_{int} \tag{2.15}$$

where W_{ex} is the elastic energy of the field of external forces (in the absence of defects), W_{def} is the sum of the energies of defects (see (2.14)) and W_{in} is the energy of interaction of elastic fields caused by defects and external forces. As will be shown below, the energy of a defect in the external field depends only on the parameters of the defect and the value of stress caused by an external field at the point $r = 0$. That is why the problem of calculating $\mathbb{W}$ may be reduced to calculation of the elastic field at points corresponding to the cores of the present defects.

Let us assume that the single defect with the elastic field (2.9) is affected by the external stress τ_{ij}. We choose the directions of the axes of the Cartesian components with reference point at $r = 0$ as

$$\begin{aligned} OX &: \vartheta = 0 \\ OY &: \vartheta = \pi/2. \end{aligned} \tag{2.16}$$

In order to calculate the energy U of interaction we use the Betti–Green formula [10]:

$$U = \int_{\mathbb{S}} W(\boldsymbol{u}, \boldsymbol{v})\,\mathrm{d}\mathbb{S} = \frac{1}{2}\int_{\partial\mathbb{S}} \boldsymbol{v}\cdot\boldsymbol{t}(\boldsymbol{u})\,\mathrm{d}(\partial\mathbb{S}). \tag{2.17}$$

Here $w(\boldsymbol{u}, \boldsymbol{v})$ is the density of energy of interaction:

$$W(\boldsymbol{u}, \boldsymbol{v}) = \tfrac{1}{2}\lambda_{ijkl}\epsilon_{ij}(\boldsymbol{u})\epsilon_{kl}(\boldsymbol{v}) \tag{2.18}$$

where $\boldsymbol{u}$ and $\boldsymbol{v}$ are the displacement vectors of the defect and the external field, respectively,

$$\boldsymbol{t}(\boldsymbol{u}) = \tau_{ij}\cos(\boldsymbol{\nu}, x_i)\,\boldsymbol{x}_j^c \qquad \tau_{ij} = \lambda_{ijkl}\epsilon_{ij}(\boldsymbol{u})$$

and $\boldsymbol{\nu}$ is the external normal vector to $\partial\mathbb{S}$.

We choose as $\partial\mathbb{S}$ the circle of radius R with the centre at $r = 0$. R is small enough to obtain

$$|R\,\mathrm{grad}(\tau_{ij})| \ll |\tau_{ij}| \tag{2.19}$$

and to regard τ_{ij} as a constant at $\partial\mathbb{S}$. After simple calculations we obtain

$$U = \pi A[c(\tau_{xx} + \tau_{yy}) + \tfrac{1}{2}(1+s)(\tau_{xx} - \tau_{yy})]/2. \tag{2.20}$$

It is possible to consider this expression as the work of the external stress at discontinuities of the displacement defined above.

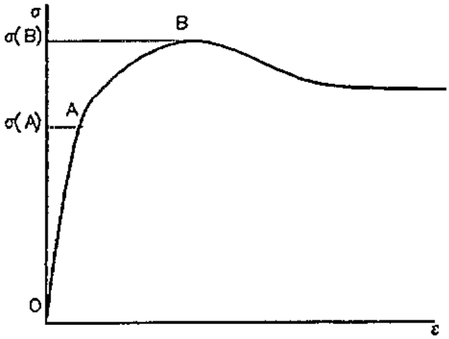

Figure 3.

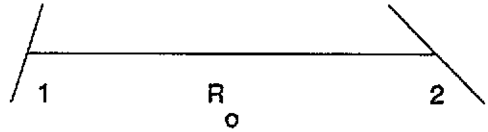

Figure 4.

3. The description of plastic phenomena

The typical behaviour of material under deformation is presented in figure 3. OA corresponds to linear elastic behaviour. The tension $\sigma(A)$ is referred to as the limit of proportionality and $\sigma(B)$ as the yielding limit of the material. BE corresponds to plastic flow.

BE is not observable in inorganic glasses under the usual conditions; fracture occurs earlier, during AB. Nevertheless, during experiments on indentation and microhardness, glasses have demonstrated plastic behaviour [11].

All the characteristic features of the deformation diagram in figure 3 may be explained and predicted with the help of the theory of defects introduced in section 2.

First we consider OA which corresponds to linear elasticity. Initially each defect present in the glass possesses a direction which corresponds to the minimum energy in a local field and which is caused by other defects. When $0 < \sigma < \sigma(A)$, the external field is too small to orient the defects. The non-linear behaviour in AB occurs because there is a sufficiently high tension to orient the present defects according to the external field with a gain in energy.

In order to estimate the limit of proportionality in the σ–ϵ diagram we consider the system in figure 4.

To calculate the energy W_{12} of interaction we use equations (2.12) and (2.20) and finally obtain

$$W_{12} = -\pi A_1 A_2(\lambda+\mu)\{2c_1c_2 - s(5-3s)[c_1\cos(2\phi_2) + c_2\cos(2\phi_1)]/2(1-s) - 2s(1+s)\cos[2(\phi_1+\phi_2)]\}/R_0^2. \tag{3.1}$$

Here A_i and c_i are the parameters of the appropriate defects, ϕ_1, and ϕ_2 are the angles between the directions of defects and the director 12, and R_0 is the distance between defects.

This system may possess several states of equilibrium. They are described by the system of equations

$$\begin{aligned} \partial W_{12}/\partial\phi_1 &= [c_2 s(3-5s)\sin(2\phi_1)]/2(1-s) + 4s(1+s)\sin[2(\phi_1+\phi_2)] = 0 \\ \partial W_{12}/\partial\phi_2 &= [c_1 s(3-5s)\sin(2\phi_2)]/2(1-s) + 4s(1+s)\sin[2(\phi_1+\phi_2)] = 0. \end{aligned} \tag{3.2}$$

It is possible to find some states of equilibrium which correspond to the minimum (states 1 and 2) and maximum (states 3 and 4) energies of interaction (figure 5). In the case of equivalent defects they are parallel in state 2 and the angle φ is expressed by

$$\cos(2\varphi) = -c(5-3s)/8(1-s^2). \tag{3.3}$$

In this case the energies of states 1 and 2 are equivalent. It provides the disordered structure of the initial defect distribution. The barrier between different structures may be roughly estimated as the difference between the energies of states 1 and 4:

$$\Delta W \simeq \pi A^2(\lambda+\mu)[4s(1+s)+cs(5-3s)/(1-s)]/R_0^2 \tag{3.4}$$

for the case of equivalent defects.

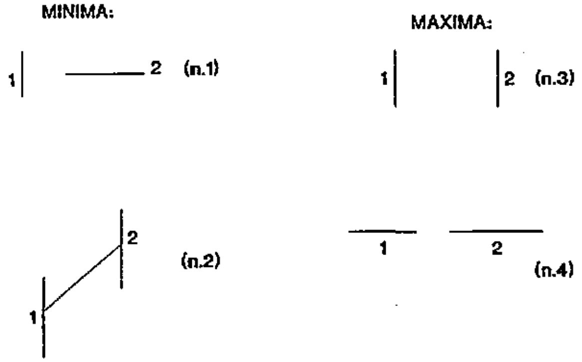

Figure 5.

The external elastic field becomes sufficient to orient the defect if energy is gained on orientation:

$$\Delta W \leqslant \sigma\pi A[c+(1+s)/2]/2 \tag{3.5}$$

where σ is the external tension.

For the limit of proportionality we have the estimate

$$\sigma^* \simeq \pi A(\lambda+\mu)[8s(1+s)+2cs(5-3s)/(1-s)]/[R_0^2(c+(1+s)/2] \tag{3.6}$$

where R_0 represents the average distance between defects. Using the data on the defect concentration [15] we may obtain the estimate

$$\sigma^*/E \simeq 5\times 10^{-3} \tag{3.7}$$

for the model of a 2D glass. Here E is Young's modulus:

$$E = (\lambda+2\mu)/(1-\nu^2)$$

where ν is Poisson's ratio.

Point B corresponds to the load $\sigma(\mathrm{B})$, which gives rise to appearance of new defects and to the growth of deformation under the constant tension, i.e. to plastic flow.

Now let us consider the case when the glass is affected by external tension ($\tau_{xx} = \sigma$; $\tau_{yy} = 0$; the fields of other defects present are neglected). The defect appears when energy is gained:

$$E_{\text{in}} < A_{\text{el}} \tag{3.8}$$

where E_{in} is the energy of the defect which appears and A_{el} is the work of the elastic field. Using for E_{in} equation (2.14) and for A_{el} equation (2.20), we finally obtain

$$\sigma = A[c^2(\lambda + 2\mu) + 2\mu(1-s)(2-s)]/[a_0^2(c + (1+s)/2)]. \tag{3.9}$$

In order to obtain the yielding limit we should find the minimum of the function $\sigma(c)$. We obtain

$$c_{\text{crit}} = [(1+s)^2/4 + 2s(1-s)(2-s)]^{1/2} - (1+s)/2 \tag{3.10}$$

and for the yielding limit

$$\sigma_{\text{min}} = 2A(\lambda + 2\mu)c_{\text{crit}}/a_0^2. \tag{3.11}$$

The next important question is that of the most suitable arrangement of the defects which appear. All of them are oriented corresponding to the external field. Now it is necessary to take into account the energy of interaction. We have established above that for the system of two parallel and equivalent defects the minimum energy of interaction corresponds to state 2 in figure 5. The critical angle ϕ_0 is now expressed as (see (3.5))

$$\cos(2\phi_0) = -c(5-3s)/8(1-s^2) \tag{3.12}$$

where $c = c_{\text{crit}}(s)$ (see (3.3)).

So, we may conclude that defects which appear in a 2D glass are aligned along the lines having an angle ϕ_0 to the direction of external force. These lines may be associated with the shear bands which do occur in materials when they are plastically deformed.

Moreover, if we consider the physical Poisson's ratio range

$$0 < \nu < 1 \qquad \text{(for two dimensions!)} \tag{3.14}$$

we obtain for c_{crit} ($\nu = 1 - 2s$)

$$0 \leqslant c_{\text{crit}} \leqslant 0.42. \tag{3.15}$$

So we obtain that, under unidirectional tension, defects appear which have a negative discontinuity of displacement in the direction normal to that of tension (see (2.10*a*) and (2.10*b*)). This leads us to the well known result that during plastic deformation a 'neck' in the specimen may appear.

Certainly, the results presented here are to be considered as a rough approximation. For simplicity we did not take into account here the energy of the core of the defect, the statistics of the system of defects, etc. Obviously all these cannot affect the qualitative results presented here.

4. Discussion

First we can compare the result for the yielding limit with the experimental data. From (3.4) we obtain

$$\sigma_{\min}/E = 2Ac_{\rm crit}/(1-\nu^2)a_0^2. \tag{4.1}$$

The estimate for $\nu = 0.4$ and for $A/a_0^2 = 0.1/(1+c)$ (see (2.10*c*)) gives

$$\sigma_{\min}/E \simeq 0.07. \tag{4.2}$$

Experiments give $\sigma_{\min}/E$-values of the order of 0.05–0.08 for various glasses [11].

Another 'control test' for our results is a comparison with the calculations in [6]. In this work the stressing is bidirectional; the 'specimen' (computer model) is loaded in two perpendicular directions. The formula for $c_{\rm crit}$ is somewhat changed:

$$c'_{\rm crit} = [(1+s)^2\chi^2/4 + 2s(1-s)(2-s)]^{1/2} - (1+s)\chi/2 \tag{4.3}$$

where χ is the yielding limit for the ratio $(\sigma_1 - \sigma_2)/(\sigma_1 + \sigma_2)$ (σ_1 and σ_2 are the tensions in perpendicular directions). For χ the following value was obtained:

$$\chi \simeq 0.64. \tag{4.4}$$

In order to estimate the angle between the shear bands and direction 1 of loading we use equations (3.6), (4.4) and (4.5) and for $\nu = 0.3$–0.5 we obtain

$$\phi_0 \simeq 49\text{–}56^\circ.$$

From the numerical experiment,

$$\phi_0 \simeq 52\text{–}55^\circ$$

to the direction of the large axis.

Unfortunately the data presented in [6] do not give us an opportunity to estimate Poisson's ratio more accurately. Nevertheless the theory developed gives quite a reliable prediction.

Also, when considering the reduced system of equilibrium equations (2.7) without any additional symmetry condition such as (2.8), only one basic solution appears in addition to (2.9):

$$\begin{pmatrix} u_R \\ u_\vartheta \end{pmatrix} = \begin{pmatrix} 0 \\ d/R \end{pmatrix} \tag{4.5}$$

which coincides with the vortex-like structure discovered in [14] by numerical simulation of plastic deformation in a 2D glass.

Acknowledgments

We are very grateful to Professor A A Berlin and to Dr V V Ginzburg for useful discussions.

References

[1] Kosevitch A M 1978 *Dislocations in the Theory of Elasticity* (Kiev: Naukova Dumka) (in Russian)
[2] Gilman 1969 *Physics of Strength and Plasticity* ed Argon (Cambridge, MA: MIT Press)
[3] Rivier N and Duffy D M 1982 *J. Physique* **43** 293–306
[4] Rivier N and Duffy D M 1981 *Proc. Colloq. on Numerical Methods in the Study of Critical Phenomena (Carry-le-Rouet, 2–4 June 1980)* (Berlin: Springer)
[5] Argon and Kuo 1979 *Mater. Sci. Eng.* **39** 101–9
[6] Berlin A A, Rothenburg L and Bathurst R J 1991 *Chim. Phys.* **10** (in Russian)
[7] Ziman J M 1979 *Models of Disorder* (Cambridge: Cambridge University Press) and references therein
[8] Klinger M I 1987 *J. Non-Cryst. Solids* **90** 29–36
[9] Porai-Koshits E A 1990 *J. Non-Cryst. Solids* **123** 1–13
[10] Mikhlin S G 1952 *Minimum Problem of the Quadric Functional* (Moscow: Gostechizdat) (in Russian)
[11] Sanditov D S and Bartenev G M 1982 *Physical Properties of Disordered Systems* (Moscow: Nauka) (in Russian)
[12] Cohen M H and Grest G S 1979 *Phys. Rev.* B **20** 1077
[13] Nelson D R 1983 *Phys. Rev.* B **28** 5515
[14] Kotelyanski M I, Mazo M A, Oleinik E F and Grivtsov A G 1991 *Phys. Status Solidi* b **166**
[15] Schober H R and Laird B B 1991 *Mod. Phys. Lett.* B **5** 795
[16] Srolovitz, Egami and Vitek 1981 *Phys. Rev.* B **24**
[17] Landau L D and Lifshitz E M 1987 *Theory of Elasticity* (Moscow: Mir) (in Russian)
[18] Nowacky W 1979 *Theory of Elasticity* (Moscow: Mir) (in Russian)