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A model of plastic deformation and localized vibration modes in 3D glass

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Abstract. The model of plastic deformation in amorphous systems based on the concept of pointlike structural defects is investigated in the three-dimensional case. The yielding limit is calculated and the propagation of shear bands is investigated. The relation between the structural defects and the low-frequency localized vibration modes is also discussed.

1. Introduction

If dealing with microscopic models of irreversible processes in the solid state (plastic deformation, melting and many other problems) the most effective approach often is to consider the solid body as an elastic continuum with a certain type of structural defect. Well known examples of this approach are the dislocation theory of plastic deformation in crystals [2], theory of phase transitions (melting) in crystals [3] and others.

Such processes occur also in the glasses. The phenomena of plasticity in usual glasses are observed preferably in the processes of fracture [4]. In polymer glasses, however, the general picture of plasticity is observed in regular conditions [5]. Moreover, in both cases it is possible to see linear structures in the deformed specimen which resemble the shear bands known from the theory of plastic deformation in crystals.

However, the attempt to consider the dislocation model of glass has not turned out to be successful [6]. The reason for the difficulties is that only in the case of a weakly disturbed crystal (i.e. if the long-range order is still conserved) is it possible to relate the real structure of the specimen to a certain distribution of dislocations and to calculate their elastic energy. In the case of the glass, however, it is not straightforward either to define the topological defects (the topology is complicated) on to calculate the elastic field of any defect defined (long-range order is absent and it seems impossible to define values similar to Burgers or Frank vectors).

A description of the topological defects in the random networks and glasses has been proposed in [7, 8]. The defects considered there are in fact chains of odd-numbered rings which either end on the surface or form closed loops. In this model the 'ground state' is the system with perfect topology (without odd-numbered rings). The elastic energy of a continuum with such defects has been calculated [7] in the semidilute approximation, i.e. in the case of large loops situated with comparatively small interloop distance. The field of the defect line is proposed to be of the same decrease rate as in the case of the dislocation (the latter is considered in the framework of the continual theory of elasticity without any connection with the microscopic structure of the solid). In such a sense the disclination

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field is supposed to be 'screened' by some dislocation distribution. This approximation turns out to be very useful—it gives us an opportunity to explain the relaxation properties in the vicinity of the glass transition and some other experimental facts.

However, for the case of the plastic deformation this approximation does not seem to be relevant. The problem is that in order to describe the plasticity we need either the motion mechanism for the structural defects (such as slip planes for the dislocations in crystals) or the possibility for the defects to appear in the system. Neither of these possibilities exist for large loops. The motion of any defect in the glass is constrained by large barriers—the 'easy motion' directions are absent. The large loops also cannot appear—such processes need huge energy. The only topological defect which may appear in the glass at low temperature is a loop of small size, involving several spheres of coordination only. From the viewpoint of the theory of elasticity it should be treated as a pointlike defect. Such a structure pattern may be a candidate for a participation in the process of plasticity.

There exist three groups of experimental facts which support the idea of pointlike structural defects responsible for the deformation processes in glasses. The first one is the experiment on bubble models of glass [9] which has demonstrated that the deformation is mainly concentrated in 'small rings' of the bubbles. The numerical simulation of a mechanical model of glass [10] has shown that the deformation is concentrated in the regions with abnormally low number of contacts between particles. These 'small rings' or regions with low number of the contacts may serve as a basis for the idea of pointlike structural defects in the glass.

The other important evidence of this concept is the well known set of anomalous thermal properties of glasses at low temperatures [11]. The theoretical explanations of these phenomena involve the 'low-frequency localized vibration modes' or 'states with double-well potential' which are responsible for these anomalies. The excitations of these modes give rise to the abnormal value and thermal dependence of the heat capacity and the scattering of regular phonons on these structures, i.e. to anomalies in the heat conductivity. Although these effects have been studied widely and for a long time [7, 11–13], their connection with the mechanical properties of the glass remains still unclear.

On the other hand, the numerical simulation [12, 13] reveals localized vibration states in the 3D model of glass. It has been demonstrated [12, 13] that these states really exist and they are connected with local structures different significantly from the average one. Normally only one abnormal vibration mode (the preferable direction of atomic mobility) is peculiar for such a local structure pattern.

The paper [1] was devoted to the construction of the model of plastic deformation in amorphous systems for the 2D case. This model was based on a concept of a structural defect similar to those developed in the present paper. The results of the 2D considerations turned out to be consistent with the data of the numerical simulations concerning the shear bands propagation. However, for the treatment of physical experiment data the construction of 3D theory is very much desirable. Besides, the experimental evidence of the localized vibration states comparable to the numerical simulation data belong certainly to the three-dimensional case only. The construction of 3D theory is the main goal of present paper.

The structure of this paper is as follows. In section 2 the model of the structural defect is introduced. In section 3 the process of the plastic deformation is considered. In section 4 the model of the structural defect is connected to the localized low-frequency modes and the results obtained are compared to experimental data.

2. The model of the structural defect

The regular description of some structural defect consists usually of two parts. We are to clarify what in fact is the core of the defect and how it interacts with the external fields. The speculations presented in the introduction part of this paper allow us to state that the structure of this core differs strongly from the average one. This means that the defect leads to a stress concentration and it is possible to calculate this additional elastic field.

The idea presented in the previous section leads to two conclusions concerning this matter:

(i) the defect has a localized core;

(ii) the atomic mobility in the core has one preferred direction, i.e. the elastic field of the defect is anisotropic.

The first statement means that the decrease rate of the long-range displacement field of the defect is the same as for the pointlike vacancies, i.e. R^{-2}; the second implies the anisotropy of the elastic field. For the sake of simplicity we use here the axisymmetric model of the defect only—the symmetry axis is related to the preferred motion direction mentioned before and the violations of this symmetry in the other directions are not essential for this consideration.

If writing down the equations of the theory of elasticity

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 \tag{1}$$

(the indexes satisfy the Einstein rule of summation) and if presenting the solution in spherical components

$$U(R, \varphi, \Theta) = \frac{F(\varphi, \Theta)}{R^2} \tag{2}$$

(U is the displacement vector) we obtain the following axisymmetric solution (independent of φ):

$$\begin{aligned} U_R &= \frac{A}{R^2}(C + \cos 2\Theta) \\ U_\varphi &= 0 \\ U_\Theta &= -\frac{A}{R^2}\gamma \sin 2\Theta \end{aligned} \tag{3}$$

where $\gamma = 2\mu/(3\lambda + 5\mu)$, λ and μ are the Lamé constants of the material. A and C are the constants of the defect.

In fact, the same expression may be obtained as the long-range limit if regarding the action of two equal forces applied at a certain distance and acting in opposite directions. It is easy to see that the limit $A \to 0, AC =$ constant corresponds to the conventional vacancy. In other words, the parameter C characterizes the 'vacancy' part of the elastic field of the defect.

For further use it is convenient to write down the expression for the displacement field in the component form:

$$U_i = \frac{A}{R^2}\left(\frac{x_i}{R}\left(C_0 + 2(1-\gamma)\frac{(d_k x_k)^2}{R^2}\right) + 2\gamma d_i \frac{d_k x_k}{R}\right). \tag{4}$$

In this expression $x_i, i = 1, 2, 3$, are the components of the radius vector, $x_i x_i = R^2$, $C_0 = C + 1$, d is the unit vector in the direction of the polar axis. This expression is invariant with respect to the choice of the local components.

The next step is to write down the strain tensor corresponding to this displacement field. The well known formula

$$\varepsilon_{ij} = \frac{1}{2}(U_{i,j} + U_{j,i})$$

gives in our case

$$\begin{aligned}\varepsilon_{ij} = \frac{A}{R^3}\Bigg(&\left(\delta_{ij} - \frac{3x_i x_j}{R^2}\right)\left(C_0 + 2(1-\gamma)\frac{(d_k x_k)^2}{R^2}\right)\\ &+2\gamma\left(d_i d_j - \frac{3(x_i d_j + x_j d_i)}{2R}\frac{d_k x_k}{R}\right)\\ &+4(1-\gamma)\frac{d_k x_k}{R}\left(\frac{(x_i d_j + x_j d_i)}{2R} - \frac{x_i x_j}{R^2}\frac{(d_k x_k)^2}{R^2}\right)\Bigg).\end{aligned} \tag{5}$$

Here δ_{ij} is the Kronecker symbol. The stress tensor is expressed as follows:

$$\begin{aligned}\sigma_{ij} &= \lambda Sp(\varepsilon_{ij})\delta_{ij} + 2\mu\varepsilon_{ij}\\ &= 2\frac{A}{R^3}\Bigg(\lambda\gamma\left(1 - 3\frac{(d_k x_k)^2}{R^2}\right) + \mu\Bigg(\left(\delta_{ij} - \frac{3x_i x_j}{R^2}\right)\\ &\times\left(C_0 + 2(1-\gamma)\frac{(d_k x_k)^2}{R^2}\right) + 2\gamma\left(d_i d_j - \frac{3(x_i d_j + x_j d_i)}{2R}\frac{d_k x_k}{R}\right)\\ &+4(1-\gamma)\frac{d_k x_k}{R}\left(\frac{(x_i d_j + x_j d_i)}{2R} - \frac{x_i x_j}{R^2}\frac{(d_k x_k)^2}{R^2}\right)\Bigg)\Bigg).\end{aligned} \tag{6}$$

Now it is possible to calculate the elastic energy of a single defect. According to well known relations of the theory of elasticity (see, e.g., [14]) we may obtain:

$$E_{single} = 2\pi\int_{a_0}^{\infty} R^2\,\mathrm{d}R\int_0^{\pi}\mathcal{W}\sin\Theta\,\mathrm{d}\Theta \tag{7}$$

where $\mathcal{W} = \frac{1}{2}\sigma_{ij}\varepsilon_{ij}$ is the energy density. The value a_0 is regarded as the radius of the core of the defect and is of the order of the interatomic distance.

The integration gives

$$E_{single} = \frac{\pi A^2}{a_0^3}(4\mu C_0^2 + C_0\tfrac{8}{3}\mu(1+\gamma) + \tfrac{4}{15}\gamma(8\mu + 4\lambda) + \tfrac{8}{5}\gamma^2\mu). \tag{8}$$

The whole energy of the defect is composed of two parts—the elastic energy calculated here and the energy of the core which may be roughly estimated as follows:

$$E_{core} \sim \mu a_0^3.$$

This value is of the same order as the elastic energy of the the defect. In fact, it is impossible to determine the exact size of the core a_0 and to calculate the energy of the core unless we have the microscopic model of the defect. For the simplest one- dimensional system and 2D system of equal particles interacting via the Lennard-Jones potential such models are described in [1].

For real 3D systems it is possible to construct the model of the defect for the physically significant case of polymer glass [15]. If taking advantage of the hierarchy of interactions specific for the polymer systems it turns out to be possible to establish the microscopic structure pattern related to the defect and to calculate the core size and energy. For the other cases such models have not been developed yet and we may deal with a rough estimation of the defect parameters only. The expression (8) determines the dependence of the elastic

energy of the defect on the intensity parameter A, the scale parameter a_0 and the parameter C_0, which, in its turn, defines the contribution of the dilatation in the field. It is possible to assume that the relation between the dilatation and shear energy contributions in the core of defect is the same as for the long-range field. Therefore for our calculation it is possible to use the expression (8) for the estimation of the *overall* energy of the defect if introducing the 'renormalized' values of A and a_0 taking into account the energy contribution of the core. This expression is used below. The estimation of the 'governing parameter' of the defect (the ratio A/a_0^3) for the microscopic models mentioned above gives the value of order 0.03–0.1 which is used in our estimations.

One more question of interest here is the overall dilatation caused by the defect defined. The calculation gives

$$\varepsilon_{kk} = 2\frac{A}{R^3}\gamma\left(1 - 3\frac{(d_k x_k)^2}{R^2}\right). \tag{9}$$

The averaging over all space gives zero, because $\langle (d_k x_k)^2/R^2\rangle = \langle \cos^2\Theta\rangle = \frac{1}{3}$. This means that the only source of the volume changes is the dilatation (or the 'free volume') in the core of defect. This additional volume may be roughly estimated as

$$\Delta V \sim 4C_0\frac{A^3}{a_0^6}$$

The energy of the elastic continuum with defects may be written as

$$W = \sum E_{single} + W_{ext} + W_{int} \tag{10}$$

where W_{ext} is the energy of the external elastic field and W_{int} the energy of the interaction between the defects and this field.

Now we are to calculate the energy of the interaction of the defect with external elastic field. Let us state that the defect with characteristic field (5) is effected by external elastic field σ_{ij}^0. The energy of the interaction is expressed by the well known formula:

$$W_{int} = \frac{1}{2}\int \sigma_{ij}^0\varepsilon_{ij}\,\mathrm{d}V. \tag{11}$$

This integral may be reduced to the surface one corresponding to the Betti–Green formula [16]:

$$W_{int} = \frac{1}{2}\int_\Omega U\cdot t(v)\,\mathrm{d}\Omega. \tag{12}$$

Here Ω is the surface of the volume V, v is the displacement vector connected with the external field,

$$t(v) = \sigma_{ij}\cos(\nu, x_i)x_j^0 \tag{13}$$

where ν is the unit normal external vector to the surface, x_j^0 is the unit vectors of the local coordinate system.

We choose as Ω the sphere of radius a_0 surrounding the defect and infinity. The external elastic field is supposed to be constant on this scale, i.e. the estimation

$$|a_0\,\mathrm{grad}(\sigma_{ij}^0)| \ll |\sigma_{ij}^0| \tag{14}$$

is supposed to be valid. In other terms, the changing scale of external field is greater than the characteristic size of the defect.

Simple calculations lead us to the following result:

$$W_{int} = \frac{2\pi A}{3}((C_0 + \tfrac{2}{5}(1-\gamma))Sp(\sigma_{ij}^0) + \tfrac{2}{5}(4+\gamma)\sigma_{33}) \tag{15}$$

(in the local system of coordinates!) Here the axis 3 is chosen in the direction of d.

Hence the energy of the interaction between the single defect and the external field is linear in the field components and depends on the field value at the point of the defect only. It is possible to calculate the overall energy of the interaction as a sum of the energies of the defects in the local fields, produced by each defect and by the external elastic loading.

3. The model of plastic deformation

Now it is possible to construct the model of the plastic deformation in the system considered.

The typical behaviour of most plastic systems under the external loading is presented in figure 1. The tension σ^* is referred to as the yielding limit of the material. Macroscopic yielding of this type is hardly observed in the inorganic glasses, but nevertheless the plastic properties may be explored in processes of microindentation etc.

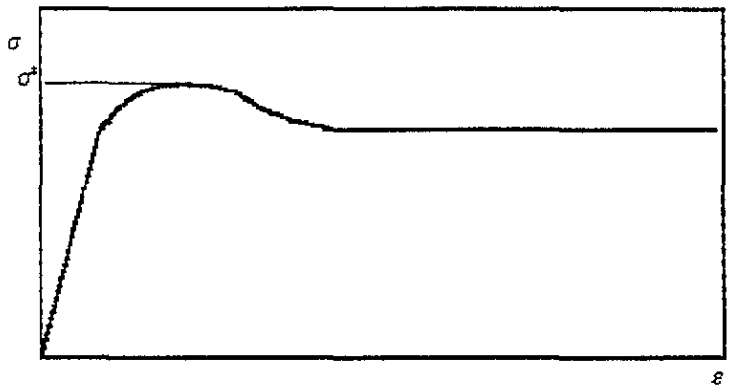

Figure 1. The typical behaviour of glass under mechanical loading (stress–strain diagram).

The characteristic features of the curve in figure 1 may be explained and predicted on the basis of the approach developed here. The explanation of the plasticity is based on the possibility of the defects appearing under external loading. The elementary act of the plastic deformation is thus the birth of the defect due to the loading. The basis of this proposition is the irreversible change in the structure and the energy dissipation in this process. The obvious criterion for this act to occur is the energy gain.

We consider the case of uniaxial loading of value $-\sigma^0$. The energy change of this system with the defect is to be less than zero:

$$\Delta W = E_{single} + W_{int} \leqslant 0. \tag{16}$$

This condition leads to following expression for the critical loading:

$$\sigma_{crit} = \frac{3A(4\mu C_0^2 + C_0 \frac{8}{3}\mu(1+\gamma) + \frac{4}{15}\gamma(8\mu + 4\lambda) + \frac{8}{5}\gamma^2\mu)}{2a_0^3(C_0+2)}. \tag{17}$$

In order to obtain the expression for the yielding limit we are to minimize the critical loading (16). This minimization gives the expression for C_0:

$$C_0 = \sqrt{4 - \frac{2a_2 - a_3}{a_1}} - 2. \tag{18}$$

In this equation $a_1 = 4\mu$, $a_2 = \frac{8}{3}\mu(1+\gamma)$, $a_3 = \frac{4}{15}(4\lambda + 8\mu) + \frac{8}{5}\gamma^2\mu$.

The yielding limit may be thus calculated as follows:

$$\sigma^* = \frac{3A}{2a_0^3}(a_2 - 4a_1 + 2\sqrt{a_1(4a_1 - 2a_2 + a_3)}). \tag{19}$$

As follows from (18), the value C_0 depends on the elastic constants of the material considered. It is dimensionless and thus it depends on the Poisson ratio ν only. For most known glasses $0 < \nu < 0.5$ and we may obtain $-0.02 < C_0 < 0.08$. As mentioned before, the value of C_0 is the measure of dilatation in the core of defect. We see that for the case of unidirectional loading the defects which preferably appear in the process of deformation realize in their vicinity the strain close to pure shear. This effect is well known and leads to appearance of the 'neck' in the zone of plastic deformation.

One more important question is the relative disposition of the appearing defects. Each defect interacts with the external field and the other present defects. In order to find the configuration corresponding to minimum of the elastic energy it is necessary to calculate the energy of interaction between the appearing defects.

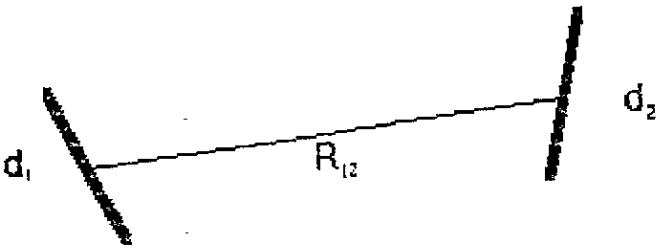

Figure 2. The respective disposition of two pointlike defects.

We characterize the relative position of two structural defects in a way demonstrated in figure 2. The values we introduce are the distance R and three angles defined by relations

$$\begin{aligned} \cos\phi_1 &= \frac{d_1 \cdot R_{12}}{R} \\ \cos\phi_2 &= \frac{d_2 \cdot R_{21}}{R} \\ \cos\Psi &= d_1 \cdot d_2. \end{aligned} \tag{20}$$

The energy of the elastic interaction between two defects may be calculated if using the relation (15) with the external field determined by the second defect in the local system of coordinates related to the first one and vice versa. Of course this calculation is valid if the distance between the defects is much more than the defect size:

$$R \ll a_0$$

In order to accomplish such calculations we need to determine the transition of the components of the stress tensor to another system of coordinates. Such a transition is governed by the well known relation [14]

$$\sigma'_{ij} = \sigma_{ij}\alpha_i\alpha_j \tag{21}$$

where α_i is the cosine of the angle between the old and new ith axis. After simple but rather lengthy calculations taking into account the relations (5), (6), (15), (20), we may

finally obtain the following expression for the energy of interaction between two defects:

$$\begin{aligned} E_{12} = \frac{2\pi A_1 A_2}{3R^3}&(2\lambda\gamma(C_{01}\tfrac{2}{5}(1-\gamma))(1-3\cos^2\phi_2) \\ &+\tfrac{2}{5}(4+\gamma)((1-3\cos^2\phi_1)(2\gamma\lambda+2\mu(C_{01}+2(1-\gamma)\cos^2\phi_1)) \\ &+4\mu\cos^2\Psi(\gamma(1-3\cos^2\phi_1)+2(1-\gamma)\cos^2\phi_1\sin^2\phi_1) \\ &+2\mu(-(\cos\Psi\cos\phi_1+\cos\phi_2)^2(3C_{01}+10(1-\gamma)\cos\phi_1^2) \\ &+\cos\Psi(\cos\Psi\cos\phi_1+\cos\phi_2) \\ &\times(3\cos\phi_1(C_{01}+2(1-\gamma)\cos^2\phi_1) \\ &-\gamma\cos\phi_1+4\gamma\cos^3\phi_1)))) + [\text{conjugation}]. \end{aligned} \tag{22}$$

In this equation the term [conjugation] denotes the same expression with *ansatz* $\phi_1 \to \phi_2$, $\phi_2 \to \phi_1$, $\Psi \to -\Psi$ and is, in fact, symmetric to the first term with respect to defects 1, 2.

The maxima and minima of this function may be determined by solving the system of equations

$$\begin{aligned} \frac{\partial E_{12}}{\partial \phi_1} &= 0 \\ \frac{\partial E_{12}}{\partial \phi_2} &= 0 \\ \frac{\partial E_{12}}{\partial \Psi} &= 0. \end{aligned} \tag{23}$$

The solution of this system of equations demonstrates the presence of a large number of equilibrium states. In order to solve the problem formulated above we need only those states which correspond to the parallel orientations of the defects. This condition implies the relations $\phi_1 = \pi - \phi_2, \Psi = 0$. For the sake of simplicity we also suppose that the appearing defects are identical and correspond to the critical value of C_0. Under these constraints the system (21) gives three different states of equilibrium:

$$\phi = 0 \tag{24a}$$

$$\phi = \frac{\pi}{2} \tag{24b}$$

$$\cos\phi_0 = \sqrt{\frac{4-7\gamma-3\mu C_0}{20(1-\gamma)}}. \tag{24c}$$

The solution (24*c*) corresponds to the energy minimum. This result means that the appearing defects tend to cooperation in lines with angle ϕ_0 to the loading direction.

In order to investigate the next stage of the cooperation process we are to study the interaction of such lines assuming that they may be considered as defects of a new type. This transition is not straightforward because we cannot describe the formation of a continuous line from single pointlike defects. We thus assume that the defects are distributed in the line with a certain density and calculate the elastic field as follows:

$$w_i = \frac{D}{A}\int_{-\infty}^{+\infty} U_i(R)\,\mathrm{d}\xi \tag{25}$$

where $D = B(3\lambda+5\mu)/4(\lambda+2\mu)$, B is the linear density of the defects, $R = \sqrt{r^2+\xi^2}$. The integration is straightforward and taking account of (4) gives

$$w_i = \frac{B}{r^2}(r_i(c_0+2(1-s)\cos^2\theta)+2e_i r s\cos\theta). \tag{26}$$

This equation is written down in the local components connected with the line, $i = 1, 2$, 3 is the direction of the line (see figure 3), $s = \mu(\lambda + 2\mu)$. The expression for the elastic field of the line is, naturally, similar to those of the elastic field of the 2D defect.

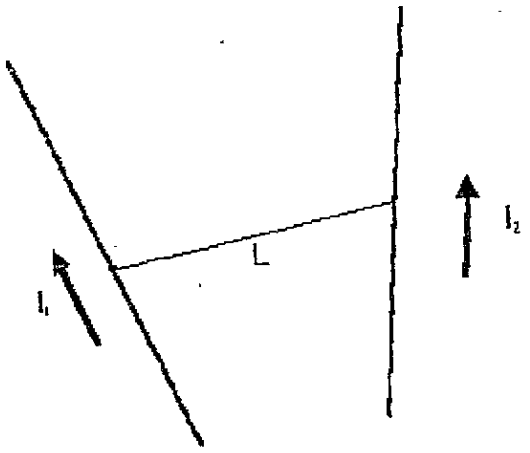

Figure 3. The respective disposition of two defect lines.

The energy of interaction between such a line and the external elastic field may be calculated with the help of the procedure described above and is expressed as follows:

$$E_{line} = \pi B \int_{-\infty}^{\infty} \mathrm{d}l \; ((C_0 + (1 - s))(\sigma_{11} + \sigma_{22}) + \tfrac{1}{2}(1 - s)(\sigma_{11} - \sigma_{22})). \quad (27)$$

The calculation gives the following expression for the energy of interaction of two identical lines:

$$W_{int} = \frac{\pi B_1 B_2}{L \sin \zeta}(F(\alpha_{ij})) \quad (28)$$

where $\zeta = l_1 \cdot l_2$ is the angle between these lines, L is the distance between lines, α_{ij} defines the respective orientation.

For the problem considered both lines are situated with angle ϕ_0 to the direction of loading. For small ζ the orientation vectors of these lines are nearly parallel. It is obvious that for the case of parallel lines the problem is reduced to the two-dimensional one. For this case it is proven [1] that there exists a linear configuration of defects with parallel orientation vectors which corresponds to the minimum of elastic energy and the energy of interaction is negative. For our 3D problem the condition $\zeta = 0$ corresponds to the singularity of the energy of interaction—this is natural due to the infinite line length. The factor of this singularity is proportional to the energy of interaction for the 2D problem and is negative for the disposition close to the energy minimum mentioned above because of the continuous character of all relations. This fact leads us to the conclusion that there exists a disposition of parallel defect lines which corresponds to the minimum of elastic energy, and in the plane transversal to the line direction it coincides with the linear structure known from the solution of the 2D problem. This means that there exists a minimum of the elastic energy which corresponds to the planar disposition of the structural defects.

Finally we may conclude that the preferred way of disposition of defects in the process of plastic deformation is to form planes. These planes are probably connected with shear bands which are well known from experiments concerning the plasticity in various amorphous systems.

As mentioned above, the consideration presented here is rather rough. We suppose, however, that a more rigorous approach will not change the qualitative conclusions of this paper.

The angle of propagation of shear bands (being the important value which may be evaluated on the basis of straightforward experiments) may be calculated exactly for the two-dimensional problem [1]. Since the defects tend to cooperate in the planes, the problem of definition of the angle of shear bands propagation is effectively two dimensional and the answer will be the same as in the paper [1].

4. The pointlike defects and low-frequency vibration modes

The results presented here demonstrate the ability of the model to describe the process of plastic deformation in amorphous systems. The question about the assumed relationship between the defects introduced and the low-frequency vibration modes remains still open. Besides, we have certain experimental data concerning these localized modes and thus it is possible to check the applicability of all our methodology taking advantage of the simple approach based on the theory of elasticity.

In order to elucidate this matter we may investigate the elastic model of the low-frequency vibrations [17].

We have to find the localized solutions of the dynamics equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} \tag{29}$$

where ρ is the average density of the system. As is well known from the theory of elasticity, the solution may be presented as

$$\boldsymbol{U} = \operatorname{grad} \Phi + \operatorname{rot} \boldsymbol{W} \tag{30}$$

where

$$\begin{aligned} &\frac{\partial^2 \boldsymbol{W}}{\partial t^2} = c_1^2 \nabla^2 \boldsymbol{W} \\ &\frac{\partial^2 \Phi}{\partial t^2} = c_2^2 \nabla^2 \Phi \\ &c_1^2 = \frac{\mu}{\rho} \qquad c_2^2 = \frac{\lambda + 2\mu}{\rho} \qquad \operatorname{div} \boldsymbol{W} = 0. \end{aligned} \tag{31}$$

If solving these equations taking account of the symmetry conditions similar to those formulated for the single stationary defect we may obtain

$$\begin{aligned} &\Phi = B\sqrt{R} Z_{5/2}(k_2 R)(3\cos 2\Theta + 1)\, \mathrm{e}^{\mathrm{i}\omega t} \\ &W_\varphi = D\sqrt{R} Z_{5/2}(k_1 R) \sin 2\Theta\, \mathrm{e}^{\mathrm{i}\omega t} \\ &W_R = W_\Theta = 0 \qquad k_1 = \frac{\omega}{c_1} \qquad k_2 = \frac{\omega}{c_2}. \end{aligned} \tag{32}$$

In this equation

$$Z_{5/2}(x) = \sqrt{\frac{2x^3}{\pi}} \left(\frac{3\cos x}{x^4} + \frac{\sin x}{x^3} - \frac{\cos x}{x^2} \right) \tag{33}$$

is the spherical Bessel function. This solution gives the growth rate of the displacement close to the centre of the excitation region equal to R^{-4}. It is obviously inconsistent with

the model of a stationary defect because it gives stronger divergence of elastic energy in the core. In order to obtain a similar type of singularity we are to assume

$$D = 3B\alpha \qquad \alpha = (k_1/k_2)^{5/2}.$$

With account of these relations we finally obtain

$$\begin{aligned} u_R &= B\left(\frac{\mathrm{d}(\sqrt{1/R}Z_{5/2}(k_2R))}{\mathrm{d}R} + 3\alpha\sqrt{\frac{1}{R^3}}Z_{5/2}(k_1R)\right)(3\cos 2\Theta + 1)\,\mathrm{e}^{\mathrm{i}\omega t} \\ u_\varphi &= 0 \\ u_\Theta &= B\left(\frac{-3\alpha}{R}\frac{\mathrm{d}(\sqrt{1/R}Z_{5/2}(k_1R))}{\mathrm{d}R} - 6\sqrt{\frac{1}{R^3}}Z_{5/2}(k_2R)\right)\sin 2\Theta\,\mathrm{e}^{\mathrm{i}\omega t}. \end{aligned} \tag{34}$$

We can estimate the size of the localization zone as the first zero of this solution. Such an estimation provides the relation between the frequency ω of vibration and the wavevector (or localization scale) of our mode. For the range of frequencies $\omega \sim 0.05\omega_0$ (here ω_0 is the characteristic frequency of optical vibrations) this estimation gives the prediction of localization zone size of order three to four spheres of coordination. This value is rather close to the numerical results of [12], [13].

This result means that the low-frequency localized modes in glasses may be successfully described with the help of the theory of elasticity even close to the core zone. We may conclude that the structural defects connected with these modes also may be described with the help of the approach based on the theory of elasticity.

5. Concluding remarks

There are several possibilities for comparing the results prescribed by the model presented here with the experimental data. It is worth while mentioning that the character of shear band growth in the mechanical model of an amorphous medium [10] was the same as prescribed by our model (i.e. new defects were born preferentially in the line formed by the previous ones). The angle of propagation of these bands also is explained by this theory (see [1] for more details).

In order to estimate the yielding limit for the particular glass we need to determine the parameters of the structural defects peculiar to this material. This is possible if constructing the microscopic model of the structural defect. For the cases mentioned above such calculation may be accomplished and it is possible to estimate the value of the yielding limit:

$$\sigma^* \sim 0.04\text{–}0.08E$$

(E is Young's modulus). This estimation turns out to be correct for most glasses.

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