

Simple description of shear dynamics of glasses with crystalline local order.

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Abstract. For those glassformers (especially metallic glasses), which structure may be presented as a set of linear topological defects embedded into a media with crystalline local order, we suggest a description of the shear dynamics in terms of kinks motion along the topological defect lines, as it is customary for crystalline materials. Locally, these defects are similar to dislocations and disclinations. For the motion of the kink, we write out the Fokker - Planck equation in a self - consistent potential. The glass transition occurs to be described as a localization of the kink.

1. Introduction

Near melting, the structure of condensed substance is often being described in terms of local order and topological defects. This approach arises from the articles [1, 2]. The base suggest of the approach is that in an overwhelming majority of local clusters of the substance (including first coordination shell) the local arrangement of the atoms is similar to the corresponding crystal arrangement, and such clusters form topologically connected area. Clusters, where the local order differs sharply from the crystalline order, are not too numerous and are organized into linear defects, which can not be terminated in the bulk of the substance. Locally, these defects are similar to dislocations and disclinations in crystal. The difference is that in globally disordered state (glass or liquid), the density of the defects is high enough to allow the disorientation of local crystalline axis at distances larger than orientational order correlation length. Since the loss of global orientation order is the main content of melting, than the approach considered implies melting being described in terms of statistics of topological defects. In two dimensions, the description of melting in terms of topological defects statistics is rather common approach [3, 4]. For three dimensions, the theory becomes mathematically complicated [5, 6], but still applicable. Melting occurs to be described as a jump rise of defect density. Recently, this approach was applied to the liquid - glass transition [7]. It is known, that metals may be transformed into nano structured (crystalline at nano scale but disordered at larger distances) state by large plastic deformation [8], i.e. by mechanical rising of topological defects density. This fact may be considered as a qualitative justification (at least for metals) of the approach considered. For the metals and alloys, the approach may be treated as a complementary to the traditional one, based on the formalism of correlation functions (for the example of the last, see [9, 10]).

In present article, we realize the following idea. In crystalline state, the shear deformation is provided by the motion of topological defects (dislocations). The last is due to the motion of point objects (kinks) along the defect line [11]. For the substance with crystalline local order, the

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same mechanism may be suggested in liquid and amorphous states also. The difference is that in the case of high defect density, the dislocation sliding plane curves into a sliding surface, and the dislocation motion is strongly retarded by the intersections with other defects. Nevertheless, the local picture of the kink motion is the same, and one can describe the shear relaxation in that terms.

2. Model of the kink motion.

Consider a certain dislocation and a certain kink moving along it. The kink's motion shifts the dislocation in its sliding surface, so the excess density of intersections with other defects occurs during the motion just behind the kink. This excess density disappears, if the kink returns conversely in a short time. Thus, if the excess intersection lifetime is infinite, the kink moves in a potential $U(x) = u_0 |x|$, where u_0 is the energy of excess intersections per unit length, and x is a coordinate along the defect line. However, the excess intersection contributes into the excess energy, so it relaxes in time, and we denote the probability to relax during time t as $m(t)$. With respect to the motion of the kink, all intersections may be divided into "excess" and "relaxed". Let us denote the probability of kink to have the coordinate below x as $F(x, t)$, and the kink probability density as $f(x, t) = F'(x, t)$. Here and below, we'll denote the derivative with respect to x by the bar, and the time derivative by the dot. It can be shown that

$$U'(x, t) = (1 - 2F(x, t))u_0(\omega_e - \omega_r), \quad (1)$$

where ω_e, ω_r are the probabilities of the intersections at (x, t) to be "excess" or "relaxed" respectively. Let us write out the equation on $\omega_{e,r}$. Within a small Δt , the probability of relaxed state at point x changes as follows:

$$\omega_r = \omega_e(x, t)m(\Delta t) + \omega_r(x, t)(1 - f(x, t)\Delta t). \quad (2)$$

Here, the first term corresponds to the relaxation from the excess to relaxed state, and the second describes possible excitation from relaxed state to the excess one by the kink motion across point x during the time interval $t \div t + \Delta t$. The obvious condition $\omega_e + \omega_r = 1$ gives closed equation

$$\dot{\omega}_e + \omega_e(m_0 + f(x, t)) = f(x, t), \quad m_0 = \dot{m}(t) |_{t \rightarrow 0}. \quad (3)$$

This equation may be easily solved

$$\omega_e = e^{-m_0 t - G} \int_0^t f(x, \tau) e^{m_0 \tau + G(x, \tau)} d\tau, \quad G(x, t) = \int f(x, t) dt \quad (4)$$

The probability density function $f(x, t)$ obeys the Fokker - Planck equation [12]

$$\frac{T}{\gamma} f'' + \frac{1}{\gamma} (U' f)' = \dot{f}, \quad (5)$$

where T is the temperature in energy units, and γ - effective friction coefficient. Relations (1,4,5) together with the condition $\omega_e + \omega_r = 1$ form a closed set of equations on the kink's distribution function $F(x, t)$. The initial condition is that at $t = 0$ the kink is at point $x = 0$. Below, we'll consider its stationary solution.

3. Stationary solution

For stationary solution, $f(x, t) = f(x)$, $\dot{\omega}_e = 0$, so that from (3) one gets

$$\omega_e = \frac{f(x)}{m_0 + f(x)}. \quad (6)$$

Equation (5) may be once integrated with respect to x :

$$\frac{T}{\gamma}F'' + \frac{u_0}{\gamma}(1-2F)F'\frac{F'-m_0}{F'+m_0} = 0. \quad (7)$$

Using standard substitution $F'' = F'dF'/dF$, one arrives to the equation

$$F' \left[\frac{dF'}{dF} + \frac{u_0}{T}(1-2F)\frac{F'-m_0}{F'+m_0} \right] = 0, \quad (8)$$

which has trivial solution $F' = 0 = f(x)$. This solution corresponds to the vanishing homogeneous distribution of the kink along the defect line. Besides, there is nontrivial solution

$$F' + 2m_0 \ln \left(\frac{m_0 - F'}{m_0} \right) = \frac{u_0}{T}(F^2 - F). \quad (9)$$

Here, we choose the integration constant as to fulfil the condition $F' = 0$ when $F = 0$ ($x \rightarrow -\infty$) or $F = 1$ ($x \rightarrow +\infty$). Let us analyze the solution of (9) at small x , where the $F(x)$ may be expanded into power series:

$$F = \frac{1}{2} + \alpha x - \beta x^3. \quad (10)$$

Using (9), one gets equations on the α, β coefficients:

$$\alpha + \frac{u_0}{4T} = -2m_0 \ln \left(1 - \frac{\alpha}{m_0} \right), \quad \beta = \frac{\alpha^2 u_0 (m_0 - \alpha)}{3T(m_0 + \alpha)}. \quad (11)$$

At large x , one can use the smallness of the F' . In that case, linear approximation of the logarithm in (9) gives

$$F = \frac{1}{2} + \frac{1}{2} \tanh \left(\frac{u_0}{2T} x \right). \quad (12)$$

Note, that nontrivial solution exists only if smooth stitching of approximations (11) and (12) at some intermediate x is possible. In the first case, the probability density function $f(x) = F'(x)$ is a parabolic cupola which width is

$$\Delta x_1 \simeq \sqrt{\frac{2T(m_0 + \alpha)}{\alpha u_0(m_0 - \alpha)}}. \quad (13)$$

In the second case, the probability density is described by the exponential cupola

$$f(x) = \frac{u_0}{4T} \cosh^{-2} \frac{u_0 x}{2T} \quad (14)$$

with the width

$$\Delta x_2 \simeq 4T/u_0. \quad (15)$$

The smooth stitching is possible if $\Delta x_1 \geq \Delta x_2$. Equations (11,13,15) give the parameters values, which correspond to the appearance of the nontrivial solution:

$$\frac{u_0}{Tm_0} = z, \quad \frac{\alpha}{m_0} = y, \quad (16)$$

where z, y are the solutions of the algebraic system

$$\begin{cases} 8y(1-y)/(1+y) = z \\ y + z/4 = -2/\ln(1-y) \end{cases} \quad (17)$$

4. Conclusion

Our reasoning may be supplemented by one natural consideration. The kink motion causes shifting of the dislocation in its sliding surface. Thus, the intersection with another defect, arising due to this shift (excess intersection), looks as a local shift of the line of this another defect according to the Burgers vector of initial dislocation, i.e. it is a kink on the another defect line. Thus, the process of its relaxation is a diffusion of this kink out from the place of intersection, which is the Poisson random process

$$m(t) = 1 - e^{-\lambda t}, \quad (18)$$

where λ is the probability of the kink to move out from the initial position per unit time, which is the half of the diffusion coefficient in the Fokker - Planck equation (5): $\lambda = 2T/\gamma$. Thus, one gets

$$m_0 = \lambda = 2T/\gamma. \quad (19)$$

Relations (16), which correspond to the point of appearance (or disappearance) of non - trivial solution, give

$$T_c = \sqrt{\frac{u_0 \gamma}{2z}}. \quad (20)$$

Above T_c , the kink moves along the defect line fluently, and shear deformations may relax (liquid). Below T_c , the kink is localized at the length $l \simeq 4T/u_0$ counted along the defect, or at the three dimensional area of size

$$r_l \sim l^d \sim T^d, \quad (21)$$

where d is the fractal dimensionality of the defect line (glass with finite shear rigidity). To produce plastic flow, one has to provide relative shear deformation $\varepsilon \sim 1/r_l \sim T^{-d}$. Measuring temperature dependence of plastic deformation, one gets fractal dimensionality of defects.

T_c in (20), is the temperature of glass instability. The effective friction coefficient γ is proportional to the viscosity, while the density of intersections u_0 is proportional to the activation energy of viscose flow. Thus, the viscosimetry experiment in the liquid state gives the T_c .

Thus, we suggested relatively simple approach which allows one to get an interesting results concerning shear dynamics of glassformers.

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