The mean velocities and densities were 1507 m/sec and 2752 kg/m^3 for VU1 and 1108 m/sec and 2386 kg/m^3 correspondingly for VU2.

NOTATION

z) symmetry axis; r) radial coordinate; ρ) density; p) pressure; U) mass velocity along z coordinate; V) mass velocity along z; E) energy; D) detonation speed; α) exponential coefficient; t) working time; τ) time segment. Subscripts denoting parameters: i) number of working cells along z; j) number of working cells along r; n) time step number; f) flow, af) approximation factor; a) activation; ip) initial powder parameters; e) explosive. A bar above a symbol denotes the dimensionless form.

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MECHANISM AND FUNCTIONAL RELATIONS CHARACTERIZING THE INFLUENCE OF AMBIENT NOISE ON THE VITRIFICATION OF GLASS-FORMING SEMICONDUCTOR MELTS

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The influence of a random temperature field applied to a melt during the cooling process on the structure and properties of disordered materials is investigated. The functional relations established in the study are explained on the basis of the microinhomogeneous structure of the melts and the strongly nonlinear behavior of internal fluctuations in transition to the nonequilibrium state.

We have previously [1-4] proposed a synergetic approach to the study of vitrification processes during the cooling of melts of glass-forming semiconductors, based on allowance for the highly nonlinear dynamics of the internal fluctuations of the system (fluctuations of the fraction of atoms in fluidlike stats and of the rms atomic displacements). These random fluctuations are insignificant under cooling conditions $q < q_c$ (q_c is the critical cooling velocity [1]), but are intensified outside the domain of stability of the equilibrium crystalline state ($q \geq q_c$), so that the mean fluctuation levels exhibit appreciable macroscopic variations [1-3]. However, the parameters describing a glass-forming melt dur-

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ing cooling vary as a result of mutual heat transfer with the environment and are therefore fluctuating quantities as well. These fluctuations can be controlled and treated as "ambient noise." Environmental fluctuations, for example, variations of the cooling rate of the melt, can affect vitrification and, more important, can generate qualitatively new nonequilibrium transitions, which are unpredictable within the framework of deterministic laws governing the evolution of the melt. In the present article we discuss aspects of the influence of ambient noise on the way in which vitrification of the melts take place.

The formation of a vitreous structure can be modeled by a bifurcation process, which is characterized by the solution of the nonlinear differential equation [1]

$$\frac{\partial\eta}{\partial t}=-\frac{\delta\Psi}{\delta t},\quad \Psi(t)=\int\left(-\frac{\lambda}{2}\eta^2-\frac{\gamma}{3}\eta^3+\frac{\beta}{4}\eta^4+\frac{G}{2}(\nabla\eta)^2\right)dx, \tag{1}$$

where x is the space coordinate, and η is the deviation of the system from the equilibrium state, which corresponds to zero variation of $\Psi(t)$ (the parameter η is interpreted as the deviation of the fraction of atoms of the nonequilibrium system in fluidlike, or amorphized, states from the fraction of such atoms in the equilibrium system); the control parameter of the system in the cooling process can be approximated by the expression [1] $\lambda = a\tilde{q}$, $a > 0$, $\tilde{q} = (q - q_c)/q_c$. The deterministic equation of motion for the parameter η has the following form on the basis of Eq. (1), ignoring spatial fluctuations:

$$\frac{\partial\eta}{\partial t}=\lambda g(\eta)+h(\eta),\quad g(\eta)=\eta,\quad h(\eta)=\gamma\eta^2-\beta\eta^3. \tag{2}$$

We assume that an external random temperature field ξ_t of intensity σ acts on the system, i.e., on the vitreous melt, during cooling. We examine the behavior of the system when the fluctuations relative to the mean cooling rate are fast enough that the Gaussian white noise approximation can be used [1], i.e., we assume that $\lambda_t = \lambda + \sigma\xi_t$. In this case the basic equation (2) reduces to a stochastic differential equation, which is written as follows in Stratonovich's interpretation:

$$d\eta(t)=(\lambda\eta+\gamma\eta^2-\beta\eta^3)\,dt+\sigma\eta\,dW_t. \tag{3}$$

Here $dW_t = \xi_1 dt$ denotes stationary increments of the random variable ξ_t, and the evolution of the probability density function $P(\eta, t)$ of η is given:

$$\partial_t P(\eta,t)=-\partial_\eta\left[\left(\lambda\eta+\gamma\eta^2-\beta\eta^3+\frac{\sigma^2}{2}\eta\right)P(\eta,t)\right]+\frac{\sigma^2}{2}\partial_{\eta\eta}\eta^2P(\eta,t). \tag{4}$$

The stationary density function $P_s(\eta)$, for which $\partial_t P(\eta, t) = 0$ and the behavior of the system relaxes to the steady state, is given by the functional relation

$$P_s(\eta)=Ng^{-1}(\eta)\exp\left(\frac{2}{\sigma^2}\int^{\eta}\frac{\lambda g(u)+h(u)}{g^2(u)}du\right)=N\eta^{\frac{2\lambda}{\sigma^2}-1}\exp\left(\frac{2\gamma}{\sigma^2}\eta-\frac{\beta}{\sigma^2}\eta^2\right). \tag{5}$$

Here N is a normalization factor, which is evaluated on the basis of the normalization condition $\int_0^\infty P_s(\eta)\,d\eta=1$:

$$N^{-1}=\int_0^\infty\eta^{2\lambda/\sigma^2-1}e^{\frac{2\gamma}{\sigma^2}\eta-\frac{\beta}{\sigma^2}\eta^2}d\eta=\frac{1}{2}\left(\frac{\sigma^2}{\beta}\right)^{\frac{\lambda}{\sigma^2}}\Gamma\left(\frac{\lambda}{\sigma^2}\right)+\frac{\gamma}{\sigma^2}\left(\frac{\sigma^2}{\beta}\right)^{\frac{\lambda}{\sigma^2}+\frac{1}{2}}\Gamma\left(\frac{\lambda}{\sigma^2}+\frac{1}{2}\right), \tag{6}$$

where $\Gamma(x)$ is the gamma function. It follows from Eqs. (5) and (6) that the function $P_s(\eta)$ is integrable on the interval (0, 1), i.e., steady-state solutions exist only if $2\lambda/\sigma^2 - 1 > 1$ or $\lambda > 0$ ($q > q_c$). For $\lambda < 0$, which is equivalent to $\tilde{q} < 0$ and $q < q_c$, the density function (5) behaves like a delta function when the expression for N is taken into account.

The extrema of the stationary density function $P_s(\eta)$ correspond to macroscopic nonequilibrium steady states of the system, and the qualitative change in the form of $P_s(\eta)$ as a function of the control parameter and noise intensity σ serves as an indicator of transition. The equation used to determine the extrema of the stationary density function (5) has the form

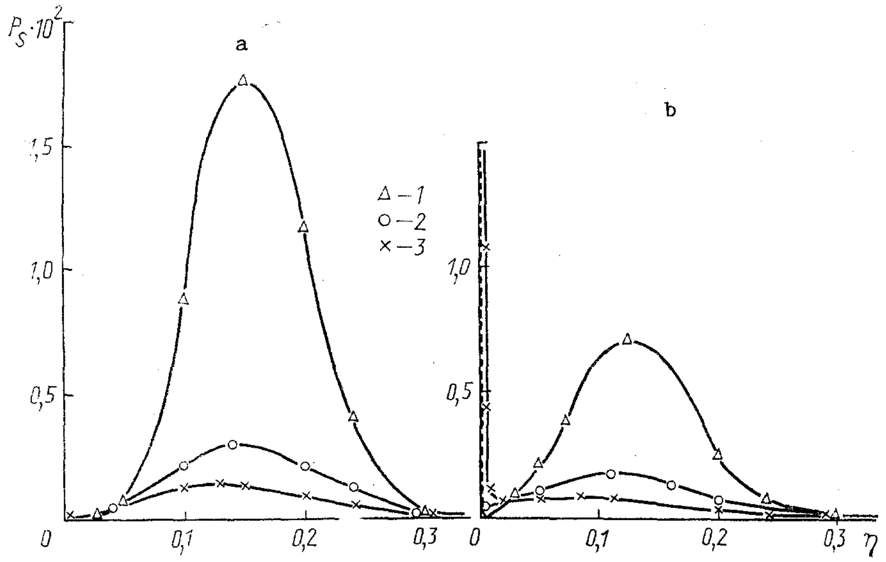

Fig. 1. Behavior of the stationary density function of fluidlike zones of a nonequilibrium system at fixed noise intensities. a) $\tilde{q} = 1.0$; b) $\tilde{q} = 0.5$; dashed curve) $\tilde{q} < 0$; 1) $\sigma^2 = 0.6$ [$\times 10^{-4}$ (K/sec^2)]; 2) 1.0; 3) 1.4.

$$\lambda\eta_m + \gamma\eta_m^2 - \beta\eta_m^3 - \frac{\sigma^2}{2}\eta_m = 0, \tag{7}$$

and its solutions are given by the relations

$$\eta_1 = 0,\ \eta_{2,3} = [\gamma \pm (\gamma^2 + 4\beta(\lambda - \sigma^2/2))^{1/2}]/2\beta.$$

The roots $\eta_{2,3}$ exist for $\lambda > \sigma^2/2 - \gamma^2/4\beta$ and always correspond to a maximum of $P_s(\eta)$, whereas η_1 corresponds to a maximum of $P_s(\eta)$ only for $0 < \lambda < \sigma^2/2$ [positive values of the deviation of the internal parameter of the system from the equilibrium state have physical significance, and so we shall analyze the curve of extrema of $P_s(\eta)$ for $\eta > 0$]. Consequently, when the melt is subjected to a random temperature field during cooling, qualitatively different transitions to the glassy state are possible. The transition for $\sigma = 0$ and $\lambda = 0$ corresponds to the deterministic case ($q = q_c$). The transition for $\sigma \neq 0$ and $\lambda = \sigma^2/2$ is accompanied by an abrupt change in the form of the density function, the deltaform distribution $P_s(\eta)$ spreading toward nonzero value of η.

The behavior of the stationary density function of the deviation of the fraction of atoms in fluidlike (amorphized) states from their equilibrium values as a function of the ambient noise intensity is shown in Figs. 1 and 2 (the calculations are carried out for $\gamma/\beta = 0.11$ and $a/\beta = 0.099$ [1]). The density function exhibits the following characteristics. If the cooling rate of the melt is below critical ($\lambda < 0$), the stationary point $\eta = 0$ corresponding to the crystalline state is asymptotically stable [in which case the distribution $P_s(\eta)$ behaves like a delta function, as represented by the dashed line in Fig. 1b]. In the presence of ambient noise and for a control parameter $0 < \lambda < \sigma^2/2$ the stationary density function becomes infinite in the limit $\eta \to 0$, i.e., some of the properties of the delta function are retained, and $\eta = 0$ is still the most probable value (Fig. 1b), but it is no longer a stable stationary point. In this case, therefore, we have a transition to a partially disordered state, which relaxes to the equilibrium state in the limit $t \to \infty$; the formation of a nonequilibrium structure is also possible, since $P_s(\eta) \neq 0$ for $\eta \neq 0$, but is it not asymptotically stable. In other words, the random temperature field has a disorganizing effect on the melt during cooling, partially disrupting the self-consistent interaction of the subsystems [2, 3]. If $\lambda = \sigma^2/2$, the nature of the distribution again changes abruptly: Even though a nonzero density function $P_s(\eta)$ exists for $\eta = 0$, the most probable value of $P_s(\eta)$ occurs for $\eta \neq 0$, for example, as represented by curve 2 in Fig. 1b. For $\lambda > \sigma^2/2$ the probability of the formation of a crystal-like structure tends to zero (Fig. 1a), and a distinct nonzero extremal value of $P_s(\eta)$ is observed. The dependence of the extrema of $P_s(\eta)$ on $\tilde{q}$ can be regarded as a very specific modification of the deterministic bifurcation dia-

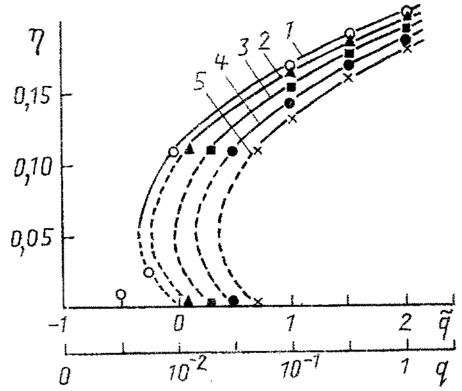

Fig. 2. Extrema of the stationary density function $P_s(\eta)$ vs cooling rate $\tilde{q}$ at fixed noise intensities. 1) $\sigma^2 = 0$; 2) 0.2 [$\times 10^{-4}$ (K/sec)^2]; 3) 0.6; 4) 1.0; 5) 1.4. q, K/sec.

gram (Fig. 2, curve 1), for which the curve $\eta(\tilde{q})$ is observed to shift with respect to $\tilde{q}$ by the amount $\sigma^2/2$ (Fig. 2, curves 2-5).

The above-described behavior of the distribution $P_s(\eta)$ leads to the following conclusion: Transition can be instigated in a glass-forming semiconductor melt during cooling by maintaining a constant mean cooling rate, but increasing or decreasing the intensity of the fluctuations of the environmental temperature field. Knowledge of only one mean state of the medium is insufficient for predicting the macroscopic behavior of the system. Indeed, for a fixed mean cooling rate, when $\lambda > \sigma^2/2$, we have $P_s(0) = 0$, the function $P_s(0)$ remains finite for $\lambda = \sigma^2/2$, and $P_s(0) \to \infty$ for $\lambda < \sigma^2/2$, i.e., the transition to a vitreous structure vanishes. Another distinct feature of noise-induced transitions, in contrast with the deterministic case, is the possible existence of a set of values of η and, accordingly, the existence of spatially disordered structures with different ordering zones.

Thus, the proposed approach can be used to calculate the critical parameter fluctuations for which the structure characterized by synthesized vitreous materials remain invariant as their production conditions vary, and also to predict the formation of qualitatively new structures at certain noise intensities.

NOTATION

q, cooling rate; ξ_t, random temperature field; σ, intensity of external temperature field; Ψ, Lyapunov functional; t, time; $P(\eta, t)$, probability density function of η.

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