# Domain structure of a new type near a photostimulated phase transition; autosolitons

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Domains of an autosoliton type can arise near a phase transition in a semiconductor subjected to intense illumination because of a redistribution of electrons in trapping levels.

The electron and lattice subsystems of ferroelectric semiconductors affect each other strongly near photostimulated phase transitions. These effects are reflected in such phenomena as an oscillation of the interface in SbSI (Ref. 1) and oscillations of the order parameter in proustite[2] ($Ag_3AsS_3$). It has been found possible to use the model proposed in Ref. 3 to describe the distinct dynamic behavior of ferroelectric semiconductors and to bring out particular features of the synergistic behavior of this system. In addition to the dynamic states mentioned above, a synergistic system may have some inhomogeneous states which are associated with a spatial correlation in the behavior of the interacting subsystems. In this letter we examine the onset of autosoliton states in ferroelectric semiconductors subjected to intense illumination.

The mutual effects of the electron and lattice subsystems in a ferroelectric semiconductor are manifested (on the one hand) in a shift of the temperature of a phase transition as a result of a variation of the electron concentration in trapping centers and (on the other) in a change in the energy intervals of the electron spectrum as a result of a change in the value of an order parameter.[3]

We write the equation describing the dynamics of the order parameter as a Landau–Khalatnikov relaxation equation:

$$\frac{d\eta}{dt} = -\Gamma\left[(\alpha + am)\eta + \beta\eta^3 + \gamma\eta^5 - \delta\frac{\partial^2\eta}{\partial x^2}\right]. \tag{1}$$

Here $\alpha$, $\beta$, $\gamma$, and $\delta$ are coefficients of an expansion of the lattice part of the thermodynamic potential in powers of the order parameter and its derivative $[\alpha = \alpha'(T - T_0)]$, $\Gamma$ is a kinetic coefficient, $\eta$ is the order parameter, and the term $am$ determines the shift of the phase-transition temperature as a result of electrons in trapping levels.

The dynamics of electrons in trapping levels is described by the following equation, which depends on the order parameter:

$$\frac{dm}{dt} = D\frac{\partial^2 m}{\partial x^2} - Q(\eta, m), \quad Q(\eta, m) \equiv -J(M - m) + mA(\eta),$$

$$J = \gamma_n n_0, \quad A(\eta) = \gamma_n N_c \exp\left(-\frac{u_0 + \tilde{a}\eta^2}{kT}\right). \tag{2}$$

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Here $n_0$ is the density of conduction electrons ($n_0 \propto I$, where $I$ is the illumination intensity), $M$ is the concentration of trapping levels, $\gamma_n$ is a kinetic coefficient, $N_c$ is the density of states in the conduction band, $u = u_0 + \tilde{a}\eta^2$ is the energy interval from the bottom of the conduction band to the trapping levels (this interval depends on the order parameter[3]), and $D$ is a diffusion coefficient.

The behavior of system (1), (2) in the homogeneous case was studied in Ref. 3. Here we wish to examine the possible appearance of, and the dynamics of, inhomogeneous states in the form of solitary domains of one phase in another phase (autosolitons). These domains would be associated with a redistribution of the electrons in trapping centers. Our system is a typical synergistic system consisting of two subsystems (the lattice and electron subsystems) which affect each other, to which the energy is supplied from the exterior. In this system, autosoliton states are realized if the sole steady state of the system is rendered metastable by the illumination. The existence of an autosoliton and the distribution of the order parameter in it are directly related to the spatial distribution of electrons in trapping centers.

The dynamics of the system is determined by the circumstances that (first) the time scales for variations in the order parameter $\eta$ and in the electron concentration in trapping centers, $m$, are quite different ($\epsilon = \tau_\eta / \tau_m \ll 1$) and (second) the typical diffusion lengths for these variables are also quite different ($\lambda = L_\eta / L_m \ll 1$). These differences mean that we can solve the problem by the method of separating fast (abrupt) processes from slow (smooth) ones.

The value of the order parameter in the region of slow motions depends on the electron concentration in trapping levels at the given point and is given by the expression

$$\eta^2 = \frac{-\beta + \sqrt{\beta^2 - 4\gamma(\alpha + am)}}{2\gamma} \equiv \eta^2(m), \quad m > m_0,$$

$$\eta = 0, \qquad m < m_0, \tag{3}$$

where $m_0$ is the concentration of electrons in traps in the vicinity of a static domain wall. This concentration is given by

$$m_0 = \frac{3\beta^2 - 16\gamma\alpha}{16\gamma a}. \tag{4}$$

The values of $m(x)$ in the region of slow motions are found from diffusion equations. The boundary conditions on these equations are specified on the basis of the following considerations. Far from an autosoliton the parameters of the system approach a uniform steady state, $\eta_s$, $m_s$, found as the steady-state solution of Eqs. (1) and (2). The values of the parameters at the center of the autosoliton, $\eta_c$, $m_c$, are found from the condition that the distribution of electrons among trapping levels at the interface is smooth. This condition is

$$\int_{m_s}^{m_0} Q(\eta(m), m) + \int_{m_c}^{m_0} Q(\eta(m), m) = 0, \tag{5}$$

where $\eta(m)$ corresponds to the value of the order parameter in the autosoliton. The half-width of the autosoliton, $L_0$, is found from $[L^2 = DA^{-1}(0)]$

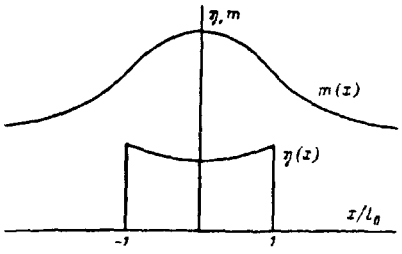


FIG. 1. Distributions of the order parameter and of the electron concentration in trapping levels in an autosoliton of the ferroelectric phase in the paraelectric phase (case *a*) ($\alpha=-21\times10^{-3}$) ($\beta=-7\times10^{4}$, $\gamma=3\times10^{10}$, $a=10^{-19}$, $\tilde{a}=4\times10^{8}$, $M=10^{18}$, $T=300$, $J=0.6$).

$$L_0=L\left(\frac{A(0)}{2}\right)^{1/2}\int_{m_c}^{m_0}\left[\int_{m_c}^{m}Q(\eta(m),m)dm\right]^{1/2}dm, \tag{6}$$

where $L$ is a characteristic diffusion length of the electron subsystem.

In a region of a rapid (abrupt) variation in the order parameter in a domain wall, at a constant $m_0$, there exists an exact solution:[5,6]

$$\eta^2=\frac{\eta_0^2}{1+\exp(-\xi/\Delta)}, \quad \Delta=\left(-\frac{4\delta\gamma}{3\beta^2}\right)^{1/2},$$

$$\eta_0^2=-\frac{3\beta^2}{4\gamma}, \quad \xi=x-x_0, \tag{7}$$

where $x_0$ is the center of the domain wall ($x_0=\pm L_0$), and $\xi$ is reckoned from the center of the corresponding domain wall.

In the region of slow motion, we find the distributions of electrons among trapping levels by integrating the steady-state part of Eq. 2:

$$|x|=L(A(0)/2)^{1/2}\int_{m_c}^{m}\left[\int_{m_c}^{m}Q(\eta(m),m)dm\right]^{-1/2}dm, \quad 0<|x|<L_0,$$

$$|x|-L_0=L(A(0)/2)^{1/2}\int_{m_0}^{m}\left[\int_{m_s}^{m}Q(\eta(m),m)dm\right]^{-1/2}dm, \quad L_0<|x|<\infty. \tag{8}$$

Since Eqs. (5)–(8) cannot be completely solved analytically, we found the final results through a numerical integration. Figure 1 shows distributions of the order parameter $\eta$ and of the electron concentration $m$ in the traps in an autosoliton for the case of an autosoliton of the ferroelectric phase in the paraelectric phase. Figure 2 shows the behavior of the autosoliton size $L_0$ as a function of the temperature or, more precisely, as a function of the parameter $\alpha[\alpha=\alpha'(T-T_c)]$, at a constant intensity of the external illumination ($J=0.6$).

The autosolitons described above are steady-state formations, but the parameters of our system are such ($\epsilon\ll1,\lambda\ll1$) that static autosolitons should, according to Ref. 4, transform into pulsating autosolitons. In addition, since the system is in a metastable

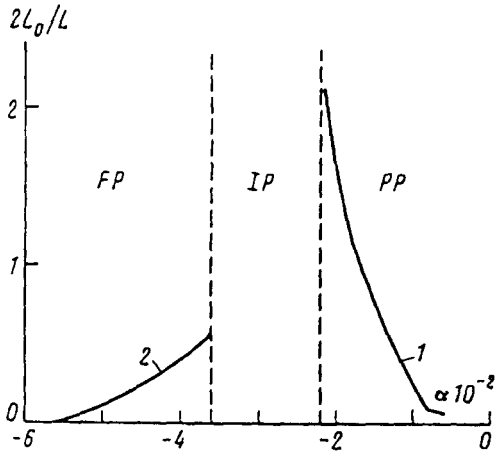


FIG. 2. Width of an autosoliton versus the parameter $\alpha[\alpha=\alpha'(T-T_c)]$. 1—For the autosoliton in Fig. 1; 2—for an autosoliton of the paraelectric phase in the ferroelectric phase. FP) Ferroelectric phase; PP) paraelectric phase; IP) unstable state. The parameter values are the same as in Fig. 1.

(flip–flop) state, a traveling autosoliton may form in it as a result of local breakdown. After this traveling autosoliton passes, the system will return to a homogeneous metastable state. The velocity of a traveling autosoliton is

$$v \approx v_0(1-\sqrt{1+\mu(m_0-m_s)}), \quad v_0 = -\beta\Gamma(\delta/\gamma)^{1/2}, \quad \mu = 4\gamma a/\beta^2. \tag{9}$$

In the case of an unstable state in the homogeneous case,[3] an autowave regime is realized in a distributed system. An autowave is a periodic domain structure of alternating ferroelectric and paraelectric phases, which is moving at a constant velocity $v_0$ [see Eq. (8)].

The evolution of an autosoliton may result in the formation of a periodic domain structure. The period would be determined by the diffusion length of the electron subsystem. This process may be a possible mechanism for the formation of the periodic domain structure which is observed in photoferroelectric materials.[7] Another mechanism for the formation of a periodic domain structure was proposed by Larkin and Khmel'nitskiĭ.[5] They link the effect with a difference between the densities of conduction electrons near an interface $[n^s/n^p = \exp(-\Delta\epsilon_g/kT)$, where $n^s$ and $n^p$ are the densities of conduction electrons in the ferroelectric and paraelectric phases, respectively]. In contrast with Ref. 5, at a high intensity of the external illumination we have $n^s \approx n^p \sim I$ ($I$ is the illumination intensity) and $n^s/n^p \approx 1$. The mechanism proposed for the formation of a domain structure in the present paper has a fundamental distinguishing feature, in addition to the obvious fact that electrons in trapping levels, rather than conduction electrons, participate in the formation of this structure. In the first place, a region of ferroelectric phase corresponds to a higher concentration of electrons in trapping centers than does a region of the paraelectric phase, in contrast with the situation in Ref. 5. The latter fact is not trivial, because an increase in the electron concentration again[5] shifts the phase transition to a lower temperature, while in the homogeneous case a relatively high concentration of electrons in trapping levels usually corresponds to the paraelectric phase, and a relatively low concentration to the ferroelectric phase. The behavior which arises is associated with the dynamics of the ferroelectric semiconductor as a whole and is an example of synergistic behavior.

In a real system, both an aperiodic domain structure and separate domains can form. The mechanism for the formation of a periodic domain structure in a real system depends on the mechanism for the realization of an autosoliton. It may involve a local breakdown at the periphery of the autosoliton, where relatively small but nonvanishing fluctuations of the order parameter are unstable,[4] or it may involve the generation of an autowave during local illumination.

In summary, we have analyzed the onset of domain formations (autosolitons) near a photostimulated phase transition. This effect is related to a self-consistent formation of domains and a nonuniform electron concentration in trapping levels (traps). The results of this study can easily be generalized to nonferroelectric structural phase transitions and to magnetic phase transitions in semiconductors.[8]

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