Memory effects in incommensurate phase in semiconductors

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(Submitted 10 July 1990)
Pis'ma Zh. Eksp. Teor. Fiz. **52**, No. 6, 952–954 (25 September 1990)

A new approach is proposed for describing memory effects in an incommensurate phase. This approach starts from the appearance of an inhomogeneous electron density at trapping levels. A correlation is established between the anomalies observed in the physical properties of crystals and the characteristics of the semiconductor subsystem.

One problem in the theory of incommensurate phases is that of describing effects in which the system remembers its state after a long hold at a certain temperature T_0. These effects are seen as anomalies in physical properties during a subsequent passage through that temperature.[1-5] Various mechanisms involving defects have been proposed to describe these effects.[6,7] In the present letter we attempt to relate these memory effects to the kinetics of the electron subsystem, to make it possible to determine the anomalies in the physical properties and the temporal characteristics of the memory from the parameters of the semiconductor subsystem.

The state of the lattice system in ferroelectric semiconductors is known to depend on the electron density m in trapping levels[8] (Fig. 1a); this point should be taken into consideration in a description of an incommensurate phase.[9] The thermodynamic po-

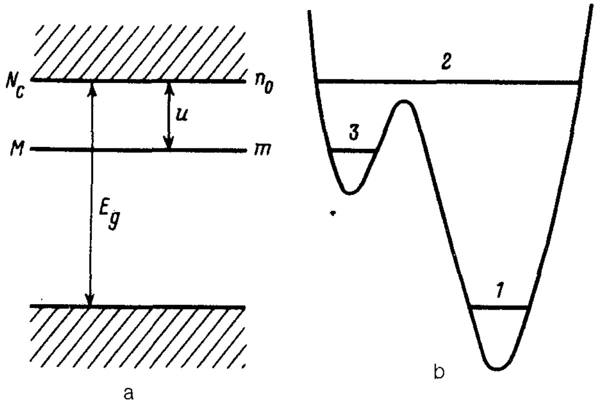

FIG. 1. a: Band structure of the semiconductor. b: Level diagram of a system with defects. 1—Ground state; 2—excited state; 3—metastable state.

0021-3640/90/180335-03$01.00

tential of a system describing an incommensurate phase can be written in the form $\Phi = \frac{1}{L}\int\bar{\Phi}dx$, where

$$\bar{\Phi} = \Phi_o + \frac{\alpha + am}{2}\eta^2 + \frac{\beta}{4}\eta^4 + \frac{\delta}{2}(\frac{\partial\eta}{\partial x})^2 + \frac{\sigma}{4}(\frac{\partial^2\eta}{\partial x^2})^2. \qquad (1)$$

Here α, β, γ, δ, σ, and κ are the coefficients of an expansion of the lattice part of the thermodynamic potential in powers of the order parameter and its derivatives $[\alpha = \alpha'(T - T_c)]$, $\eta = \rho\cos\varphi(x)$ is the order parameter, ρ and φ are the amplitude and phase of the order parameter, and the term am describes the shift of the phase-transition temperature due to the electrons in trapping levels. Since the electron density in the trapping levels, m, depends on the state of the lattice system, an inhomogeneous density of electrons in trapping levels arises in the region of the incommensurate phase or of the modulated structure, along with the homogeneous density:

$$m = m_0 + m_1(x). \qquad (2)$$

Here m_0 is the homogeneous electron density in trapping levels, and $m_1(x)$ is the inhomogeneous part. The values of the inhomogeneous and homogeneous electron densities in trapping levels are found from an equation which describes the kinetics of the electron density in the trapping levels:

$$\frac{dm}{dt} = \gamma_n n_0(M - m) - \gamma_n m N_c exp(-\frac{u_0 + \tilde{a}\eta^2}{kT}). \qquad (3)$$

Here n_0 is the density of conduction electrons, M is the density of trapping levels, γ_n is a kinetic coefficient, N_c is the density of states in the conduction band, and $u = u_0 + \tilde{a}\eta^2$ is the energy interval between the bottom of the conduction band and the trapping levels. This energy interval depends on the order parameter.[9] From (3) we find the equilibrium electron density in trapping levels:

$$m = \frac{n_0 M}{n_0 + N_c exp(-\frac{u_0 + \tilde{a}\eta^2}{kT})}, \qquad (4)$$

Under equilibrium conditions, an inhomogeneous density of electrons in trapping levels thus arises because of a modulation of thermal scattering. Expanding m in (4) in powers of the small parameter $\tilde{a}\eta^2/kT$, we find

$$m_0 = \frac{n_0 M}{n_0 + N_c exp(-\frac{u_0}{kT})}; \qquad m_1(x) \approx \frac{N_c exp(-\frac{u_0}{kT})\frac{\tilde{a}m_0}{kT}}{n_0 + N_c exp(-\frac{u_0}{kT})}\eta^2 \quad . \qquad (5)$$

The relaxation times τ_m of the electron density in trapping levels are determined by thermal scattering:

$$\tau_m = (\gamma_n(n_0 + N_c exp(-u_0/T))^{-1} \quad . \qquad (6)$$

The times τ_m are long enough to describe memory effects: With $\gamma_n = 10^{-13}$ cm^3/s, $n_0 = 10^8$–10^{10} cm^{-3}, $N_c = 10^{19}$ cm^{-3}, and $u_0/kT = 20$–25 (for proustite,[9] for example, we have $u_0 = 0.12$ eV at $T \sim 50$ K), we find $\tau_m = 5$–300 min. The average value of $m_1(x)$ in the sample is on the order of $0.15m_0$.

As the temperature is lowered, a phase transition to an incommensurate phase thus occurs. The subsequent change in $k(T)$ is accompanied by an increase in the amplitude of the order parameter. The homogeneous part of the electron density in trapping levels adjusts to the equilibrium value m_0 in (5). After a halt at a certain temperature T_0, the inhomogeneous part of the electron density in attachment levels gradually increases, causing a gradual decrease in the amplitude of the order parameter from $\rho^2 \approx -(\alpha + am_0)/\beta$ to the equilibrium value,

$$\rho_0^2 = -\frac{\alpha + am_0}{\beta + \frac{a\tilde{a}m_0}{kT}}, \tag{7}$$

Correspondingly, there are changes in other physical properties which depend on the order parameter. The system now remembers the inhomogeneous distribution of the electron density in the trapping centers with a certain value of the wave vector $k(T_0)$, even if the temperature is changed. The relaxation time of this metastable state is 5–300 min. If, after a certain time shorter than τ_m, this temperature is passed again, a bend forms on the temperature dependence of the amplitude of the order parameter. This bend corresponds to the equality of the wave vector of the structure which arises and the wave vector of the inhomogeneous distribution of electron density in the trapping centers. If we stop at this temperature, the system adjusts to the inhomogeneous distributions of electrons in the trapping centers in a short time τ_η. The system thus remembers its state. Later on, over times τ_m, there is a subsequent relaxation to ρ_0 in (6), if this value has not already been reached. Similar effects have been observed in Refs. 1–5.

The structure of the inhomogeneous electron distribution in trapping centers which arises may force the incommensurate phase to behave in the manner of a commensurate phase, since the behavior of the electron density will be correlated with the behavior of the main lattice.

This approach can be taken to describe the effects of intrinsic defects in metastable states on phase transitions (Fig. 1b), with the one new feature that the variable m will correspond to the defect concentration in the metastable state.

It follows from this analysis that memory effects in an incommensurate phase in a semiconductor are related to the appearance of an inhomogeneous electron density in trapping centers, so the application of light and other agents which would alter the population of trapping centers would have a substantial influence on memory effects.

I wish to thank G. B. Teĭtel'baum for constant interest in this study and for useful discussions.

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Translated by D. Parsons