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MICROSCOPIC THEORY OF FERROELECTRIC PHASE TRANSITIONS INDUCED BY ELECTRON-PHONON INTERACTION IN A^IV B^VI-TYPE COMPOUNDS. 1

(Presented by V. Hizhnyakov)

The microscopic theory of ferroelectric phase transitions caused by the electron-phonon interaction in A^IV B^VI-type semiconductors has been developed with the allowance made for the real electronic band structure. The Helmholtz free energy has been obtained. The electron-phonon interaction generates simultaneously the ferroelectric soft-mode, and the temperature dependent elastic and electrostrictive constants.

1. Introduction

The vibronic theory of ferroelectric phase transition (FPT) (see, e. g. [1—5]) has been successfully applied to the explanation of some experimental data on A^IV B^VI (PbTe, SnTe etc.) semiconductors [1, 3, 5—10]. In particular, the vibronic theory has predicted the influence of the magnetic field on the Curie point that has later been discovered experimentally in $Pb_xGe_{1-x}Te$ [9]. According to this theory the properties of FPT also exhibit an essential dependence on the carrier concentration [2, 5], that is observed experimentally in a number of cases [11].

The versions of the vibronic model of FPT for GeTe, proposed in [12—14], are based on a simplified band structure and, therefore, a development of the theory taking into account the real electronic band structure of these crystals [15] is necessary. In [16] the structural instability of A^IV B^VI compounds is connected with the proposed properties of

the Fermi surface $\varepsilon(k_F) \approx \varepsilon(k_F+Q)$, where $Q = \left(\dfrac{\pi}{a}\right)(1, 1, 1)$. The

electronic spectrum with such properties is related to some prototype phase (in essence such spectrum has been used in [17] for bismuth).

In this work the theory of FPT in A^IV B^VI semiconductors has been developed with the real band structure [15], electron-phonon and phonon-phonon interactions taken into account.

2. The Helmholtz Free Energy

The initial Hamiltonian of the electron-phonon system is the following (see also [7, 18]):

$$H = H_e + H_{ph} + H_{e-ph}, \qquad (1.1)$$

where

$$H_e = \sum_{\sigma,k} \varepsilon_\sigma(k) a^+_{\sigma k} a_{\sigma k} + \sum_{\sigma,\sigma'} \sum_k [P_{\sigma\sigma'}(k) a^+_{\sigma k} a_{\sigma' k} + \text{h. c.}], \qquad (1.2)$$

$$H_{ph} = \frac{1}{2} \sum_{q,j} (M_j^{-1} P_{qj} P_{-qj} + M_j \omega_{qj}^2 y_{qj} y_{-qj}) +$$

$$+ \sum_{q_1,q_2,q_3,q_4} \sum_{j_1,j_2,j_3,j_4} B \begin{pmatrix} q_1 & q_2 & q_3 & q_4 \\ j_1 & j_2 & j_3 & j_4 \end{pmatrix} y_{q_1 j_1} y_{q_2 j_2} y_{q_3 j_3} y_{q_4 j_4}, \tag{1.3}$$

$$H_{e-ph} = N_0^{-1/2} \sum_{\sigma,\sigma',j} \sum_{k,q} [V_{\sigma\sigma'}^j (q) y_{qj} + N_0^{-1/2} W_{\sigma\sigma'}^j y_{qj} y_{-qj}] a_{\sigma k}^+ a_{\sigma' k-q}. \tag{1.4}$$

Here H_e, H_{ph} and H_{e-ph} are the Hamiltonians of the electronic and phonon subsystems and of the electron-phonon interaction; $\varepsilon_\sigma(k)$ are the initial (taking into account spin-orbit interaction) spectra of the valence ($\sigma = 1, 2$) and conduction ($\sigma = 3, 4$) bands, respectively, with the wave functions $|L^6 \bar\alpha\rangle$, $|L^6 \bar\beta\rangle$ and $|L^{6'} \bar\alpha\rangle$, $|L^{6'} \bar\beta\rangle$ ($\bar\alpha$, $\bar\beta$ are the spin indices); a^+, a are electron creation and annihilation operators (k is the wave vector); y_{qj} are normal coordinates ($y_{qj} = \bar{y}_{qj} + \hat{y}_{qj}$, $\bar{y}_{qj}$ are c numbers, further the minimization parameters of the free energy, $\hat{y}_{qj}$ is the corresponding operator part), and P_{qj} are the conjugated momenta of the vibrations with the initial frequencies ω_{qj}; q is the wave vector of phonons; j is the index of the vibrational branch ($j=1$ corresponds to the ferroelectric (FE) optical vibrational branch, $j=2$, to the acoustical one), M_j are the corresponding reduced masses; V and W are the constants of linear and quadratic electron-phonon interactions; $P_{\sigma\sigma'}(k)$ are the matrix elements of kp interaction in a six-band model [15]. The last term in (1.3) describes phonon-phonon interactions (the third-order anharmonicity has been taken into account by the renormalization of B in [2, 5]); N_0 is the number of unit cells in a crystal. Hamiltonian (1.1) takes simultaneously into account electron-phonon interactions and the forming of the energetic spectra of the valence and conduction bands of $A^{IV}B^{VI}$ semiconductors.

To find the Helmholtz free energy of the system we use the electronic energetic spectra renormalized by vibronic interactions, found on the basis of Hamiltonian (1.1) in [7, 18]

$$E_{1,2}(k) = \frac{1}{2} [\tilde\varepsilon_1(k) + \tilde\varepsilon_2(k)] \mp \left\{ \left[\frac{\tilde\varepsilon_2(k) - \tilde\varepsilon_1(k)}{2} \right]^2 + \right.$$

$$+ P_\perp^2 k_\perp^2 + P_\parallel^2 k_\parallel^2 + \frac{1}{N_0} [V_\perp^2 (x_L^2 + y_L^2) + V_\parallel^2 z_L^2] + \tag{1.5}$$

$$\left. + \frac{2}{\sqrt{N_0}} [P_\parallel V_\parallel k_\parallel z_L + P_\perp V_\perp (k_x' x_L + k_y' y_L)] \right\}^{1/2},$$

where

$$\tilde\varepsilon_{1,2}(k) = \varepsilon_{1,3}^*(k) + \frac{1}{\sqrt{N_0}} [D_\perp^{(1,3)} (\varepsilon_{xx}^{(L)} + \varepsilon_{yy}^{(L)}) + \tag{1.6}$$

$$+ D_\parallel^{(1,3)} \varepsilon_{zz}^{(L)}] + \frac{1}{N_0} [W_\perp^{(1,3)} (x_L^2 + y_L^2) + W_\parallel^{(1,3)} z_L^2]$$

at this

$$\varepsilon_{1,3}^*(k) = \varepsilon_{2,4}^*(k), \qquad A_{\perp,\parallel}^{(1,3)} = A_{\perp,\parallel}^{(2,4)}, \qquad A \equiv D, W, \tag{1.7}$$

$$\varepsilon_{1,2}^*(k) = \varepsilon_{1,2}(k) - \varepsilon_{dyn}^{(1)}, \qquad \varepsilon_{3,4}^*(k) = \varepsilon_{3,4}(k) + \varepsilon_{dyn}^{(2)}. \tag{1.8}$$

Here $A_{\perp,\parallel}$ ($A \equiv P, D, V, W$) are the transverse ($\perp$) and longitudinal ($\parallel$) components of the matrix elements of the **kp** interaction between the bands L^6 and $L^{6'}$ (P), of the constants of deformation potential for acoustical vibrations (D), and of the linear interband (V) and quadratic intraband (W) electron-phonon interactions for FE optical vibrations; a_L and $\varepsilon^{(L)}_{\alpha\alpha}$ ($\alpha = x, y, z$) are the coordinates of the FE mode and the components of strains in the system of symmetry axes of L-extrema, $k_\parallel = = k_z - k_{zL}$, $k'_x = k_x - k_{xL}$, $k'_y = k_y - k_{yL}$ and $k^2_\perp = (k'_x)^2 + (k'_y)^2$. In (1.5)—(1.8) the terms $\varepsilon^{(1,2)}_{\text{dyn}}$ take into account the dynamical part of the electron-phonon interaction (the terms $\sim \hat{y}_{qj}$ in (1.1)) [7]. We go from the components $\varepsilon^{(L)}_{\alpha\alpha}$ and a_L to the corresponding components ($\varepsilon_{\alpha\alpha'}$ and $y_{1,2,3} = x, y, z$) in the system of the basic axes of the crystal. The spectra $E^{(l)}_{v=1,2}$ (the index $l = 1, 2, 3, 4$ numbers the valleys), obtained as a result of such transformation for $A^{IV}B^{VI}$-compounds, are given in [7].

On the basis of (1.1) and (1.2) the electronic part of the Helmholtz free energy of $A^{IV}B^{VI}$-compounds, renormalized by electron-phonon interactions, is obtained in the form

$$F_e = \sum_{v,l} [n^{(l)}_v \mu - k_B T Z^{(l)}_v], \tag{1.9}$$

where

$$Z^{(l)}_v = \sum_k \ln \left[1 + \exp \left(\frac{\mu - E^{(l)}_v(k)}{k_B T} \right) \right], \quad n^{(l)}_v = k_B T \frac{\partial Z^{(l)}_v}{\partial \mu}. \tag{1.10}$$

The chemical potential μ in (1.10) is determined by the condition $\sum_{v,l} n^{(l)}_v = N$, at this N is the number of electrons in the system.

To perform a thorough analysis of the picture of FPT in $A^{IV}B^{VI}$-compounds and to present the theory in a form more convenient for comparing with the experiment, we expand the electronic part of the free energy (1.9) in the powers of polarizations ($P_i \sim y_i$) and strains, and add at once the phonon part of the free energy. Taking into account the fourth-order terms, we have

$$F = \frac{\alpha_1}{2} \sum_i y^2_i + \frac{\beta_1}{4N_0} \sum_i y^4_i + \frac{\beta_2}{N_0} \sum'_{i,j} y^2_i y^2_j + \frac{\bar{c}_{11}}{2} (\varepsilon^2_{xx} + \varepsilon^2_{yy} + \varepsilon^2_{zz}) +$$

$$+ \bar{c}_{12} [\varepsilon_{xx}(\varepsilon_{yy} + \varepsilon_{zz}) + \varepsilon_{yy}\varepsilon_{zz}] + \frac{\bar{c}_{44}}{2} (\varepsilon^2_{yz} + \varepsilon^2_{xz} + \varepsilon^2_{xy}) +$$

$$\tag{1.11}$$

$$+ N^{-1/2}_0 \{ g_1(\varepsilon_{xx}x^2 + \varepsilon_{yy}y^2 + \varepsilon_{zz}z^2) + g_2 [\varepsilon_{xx}(y^2 + z^2) + \varepsilon_{yy}(x^2 + z^2) +$$

$$+ \varepsilon_{zz}(x^2 + y^2)] + g_3 (\varepsilon_{xz}xz + \varepsilon_{yz}yz + \varepsilon_{xy}xy) \},$$

where the squared FE $q = 0$ mode frequency in the paraphase is equal to

$$\alpha_1 = M\hat{\omega}^2_0 + 4 \sum_k \left\{ W^+ - \Delta f_k E_k \left[p_1(k) - \frac{2}{3} E^2_k v_1(k) \right] \right\}, \tag{1.12}$$

here the frequencies ω_0 ($\omega_{01} \equiv \omega_0$, $M_1 \equiv M$) renormalized by phonon-phonon interactions are expressed as follows [2, 5]:

382

$$\hat{\omega}_0^2 = \omega_0^2 + M^{-1} \sum_{q,j} A_j(\mathbf{q}) \, \text{cth} \, \frac{\hbar \omega_{qj}}{2k_B T},$$

$$\hat{\omega}_0^2 \approx \omega_0^2 + M^{-1} \overline{A} k_B T \quad (\text{at } 2k_B T \gg \hbar \omega_{q1,2}) \tag{1.13}$$

and

$$\Delta \hat{f}_{\mathbf{k}} = \frac{1}{2} \left[\text{th} \, \frac{E_2(\mathbf{k}) - \mu}{2k_B T} - \text{th} \, \frac{E_1(\mathbf{k}) - \mu}{2k_B T} \right], \quad E_{\mathbf{k}} = [E_2(\mathbf{k}, \alpha_L = 0, \, \varepsilon_{\alpha\alpha}^{(L)} = 0) -$$

$$- E_1(\mathbf{k}, \alpha_L = 0, \, \varepsilon_{\alpha\alpha}^{(L)} = 0)]^{-1}, \quad p_1(\mathbf{k}) = 2(W^- \Delta_{\mathbf{k}} + K_0), \tag{1.14}$$

$$\Delta_{\mathbf{k}} = \varepsilon_3(\mathbf{k}) - \varepsilon_1(\mathbf{k}), \quad K_0 = \frac{1}{3N_0} (2V_\perp^2 + V_\parallel^2), \tag{1.15}$$

$$v_1(\mathbf{k}) = \sqrt{t_1(\mathbf{k})} + \sqrt{t_3(\mathbf{k})}, \quad t_{1,3}(\mathbf{k}) = \frac{1}{N_0^2} (P_{\parallel,\perp} V_{\parallel,\perp} k_{\parallel,\perp})^4, \tag{1.16}$$

$$W^{\pm} = \frac{1}{6N_0} (2W_\perp^{\pm} + W_\parallel^{\pm}), \quad W_{\perp,\parallel}^{\pm} = W_{\perp,\parallel}^{(3)} \pm W_{\perp,\parallel}^{(1)}. \tag{1.17}$$

The quantities $A_j(\mathbf{q})$ and $\overline{A}$ in (1.13) describe the phonon anharmonicity. The coefficients of anharmonicity stabilizing the low-symmetry phases are equal to

$$\beta_1 = \frac{K}{12}, \quad \beta_2 = L + \frac{\beta_1}{2} \tag{1.18}$$

with

$$L = -2N_0 \sum_{\mathbf{k}} \Delta \hat{f}_{\mathbf{k}} E_{\mathbf{k}} \left\{ (W_1^-)^2 - \frac{1}{4} [p_2(\mathbf{k}) E_{\mathbf{k}}]^2 + \frac{p_2(\mathbf{k})}{2} \times \right.$$

$$\left. \times v_2(\mathbf{k}) E_{\mathbf{k}}^4 - \frac{5}{9} E_{\mathbf{k}}^6 \left[t_1(\mathbf{k}) + \frac{5}{4} t_3(\mathbf{k}) - 7t_4(\mathbf{k}) - 3t_2(\mathbf{k}) \right] \right\} + \eta_{1,ph} \tag{1.19}$$

and

$$K = -2N_0 \sum_{\mathbf{k}} \Delta \hat{f}_{\mathbf{k}} E_{\mathbf{k}} \left\{ 48(W^-)^2 - 3[p_1(\mathbf{k}) E_{\mathbf{k}}]^2 + 12 \times \right.$$

$$\left. \times p_1(\mathbf{k}) v_1(\mathbf{k}) E_{\mathbf{k}}^4 - 5E_{\mathbf{k}}^6 \left[\frac{1}{3} (4t_1(\mathbf{k}) + 5t_3(\mathbf{k}) + 8t_4(\mathbf{k})) + 8t_2(\mathbf{k}) \right] \right\} + \eta_{2,ph}. \tag{1.20}$$

Here

$$t_2(\mathbf{k}) = \sqrt{t_1(\mathbf{k}) t_3(\mathbf{k})}, \quad t_4(\mathbf{k}) = \frac{1}{N_0^2} (P_\perp^2 V_\perp^2 k_x k_y)^2, \tag{1.21}$$

$$p_2(\mathbf{k}) = W_1^- \Delta_{\mathbf{k}} + K_1, \quad v_2(\mathbf{k}) = 2\sqrt{t_1(\mathbf{k})} - \sqrt{t_3(\mathbf{k})}, \tag{1.22}$$

$$W_1^- = \frac{1}{3N_0} (W_\parallel^- - W_\perp^-), \quad K_1 = \frac{2}{3N_0} (V_\parallel^2 - V_\perp^2). \tag{1.23}$$

In (1.19)—(1.20) $\eta_{1,2,ph}$ take into account the contribution from phonon-phonon interactions to $\beta_{1,2}$, analogously to [2,5].

The elastic and electrostrictive constants renormalized by vibronic interactions are expressed as follows:

$$\bar{c}_{11,12} = c_{11,12} + (\Lambda^-)^2 S_1, \quad \bar{c}_{44} = c_{44} + (\Lambda_1^-)^2 S_1, \tag{1.24}$$

$$g_{1,2} = g_{a,b} + S_2, \quad g_3 = g_c - 4 \sum_k \Delta f_k E_k \Lambda_1^- \times$$

$$\times \left\{ W_1^- - \frac{1}{4} \Delta_k E_k^2 \left[p_2(k) - E_k^2 v_2(k) \right] \right\} \tag{1.25}$$

here

$$S_1 = -4 N_0^{-1} \sum_k \Delta f_k E_k \left[1 - \frac{1}{4} (\Delta_k E_k)^2 \right], \tag{1.26}$$

$$S_2 = -8 \sum_k \Delta f_k E_k \Lambda^- \left\{ W^- - \frac{1}{8} \Delta_k E_k^2 \left[p_1(k) - 2 v_1(k) E_k^2 \right] \right\} \tag{1.27}$$

and the elastic constants renormalized by phonon-phonon interactions, equal to $(\bar{B}_{\rho j}(\mathbf{q}))$, are determined by the coefficients of anharmonicity B and ω_{qj})

$$c_{11,12} = c_{11,12}^* + R_{1,2}, \quad c_{44} = c_{44}^* + R_3 \tag{1.28}$$

with

$$R_\rho = \sum_{q,j} \bar{B}_{\rho j}(\mathbf{q}) \operatorname{cth} \frac{\hbar \omega_{qj}}{2 k_B T}. \tag{1.29}$$

In (1.28), (1.25) $c_{11,12,14}^*$ and $g_{a,b,c}$ are the initial elastic and electrostrictive constants. The quantities Λ^- and Λ_1^- are determined by (1.17), (1.23) through the deformation potentials by a substitution $W \to N_0 D$.

Thus, as can be seen from (1.11)—(1.29); electron-phonon interactions generate the soft mode, the temperature dependent elastic and electrostrictive constants, and vibronic anharmonicity for the stabilization of a structural phase transitions, i.e. the free energy of $A^{IV}B^{VI}$ ferroelectric-semiconductors (1.11) contains all types of terms postulated in the phenomenological theory.

Now we shall analyse in detail the case when spontaneous strains are equal to zero. On the basis of (1.11), we obtain analogously to the phenomenological theory for the rhombohedral phase (the expressions for the spontaneous lattice distortion in other phases are omitted)

8 configurations of types
$$x_0^2 = y_0^2 = z_0^2 = -\frac{\alpha_1 N_0}{\beta_1 + 4 \beta_2}. \tag{1.30}$$

The frequency of FE mode splits in the rhombohedral phase:

$$M \Omega_z^2 = \alpha_1 + 3(\beta_1 + 4 \beta_2) \frac{x_0^2}{N_0}, \quad M \Omega_{x,y}^2 = \alpha_1 + 3 \beta_1 \frac{x_0^2}{N_0}. \tag{1.31}$$

Introducing the effective charge $\bar{e}$ [2, 5, 19] corresponding to the vibration y_i the spontaneous polarization may be written in the form

$$P_{si} = \frac{\bar{e} y_{i0}}{v \sqrt{N_0}}, \tag{1.32}$$

where $\dfrac{y_{i0}}{\sqrt{N_0}}$ are the components of the order parameter determined by

384

(1.30) and v is the volume of the unit cell. The dielectric susceptibility in high-symmetry and rhombohedral phases equals, respectively, $\chi_{hs} = \bar{e}^2 (vM\Omega_{hs}^2)^{-1}$ and $\chi_{z;\,x,y} = \bar{e}^2 (vM\Omega_{z;\,x,y}^2)^{-1}$.

3. Calculation of the Soft-Mode Frequencies

Now the soft-mode frequencies will be calculated by basing on (1.12) and taking into account the concrete form of the real spectra of the valence and conduction bands of $A^{IV}B^{VI}$ semiconductors. The initial spectra $\varepsilon_\sigma(k)$ in (1.5) are of the form [15]

$$\varepsilon_{1,2}(k) = -\frac{\hbar^2}{2}\left(\frac{k_\perp^2}{m_\perp} + \frac{k_\parallel^2}{m_\parallel}\right),$$

$$\varepsilon_{3,4}(k) = \Delta + \frac{\hbar^2}{2}\left(\frac{k_\perp^2}{m'_\perp} + \frac{k_\parallel^2}{m'_\parallel}\right), \tag{1.33}$$

where $m_{\perp,\parallel}$ and $m'_{\perp,\parallel}$ are the transverse and longitudinal components of the effective masses of electrons and holes, renormalized by $\mathbf{kp}$ interactions with other bands in a six-band model, Δ being the initial forbidden gap. We introduce the following designations —

$$M^\pm_{\perp,\parallel} = (m_{\perp,\parallel})^{-1} \pm (m'_{\perp,\parallel})^{-1}, \qquad \bar{a}_{1,2} = \frac{\hbar^2}{2}M^+_{\perp,\parallel}, \tag{1.34}$$

$$G_{1,2} = \frac{\hbar^4}{16}\left[(M^+_{\perp,\parallel})^2 - (M^-_{\perp,\parallel})^2\right], \qquad G_3 = \frac{\hbar^4}{8}(M^+_\perp M^+_\parallel - M^-_\perp M^-_\parallel). \tag{1.35}$$

First we calculate the quantity α_1 in the mean field approximation ($\varepsilon_{dyn}^{(1,2)} = 0$). Herewith we take the constants of the quadratic vibronic interaction $W = 0$ (an analysis has shown that this interaction is essential in the systems undergoing a transition to the tetragonal phase) and $\Delta f_k(T) \approx \Delta f_k(0) = 1$. The case of degenerate semiconductor will be considered below. Besides, we neglect the term containing $G_{1,2,3}$ in (1.5), i.e. in the absence of electron-phonon interactions (1.5) are the spectra of Martinez type [15]. The sums in (1.12) can be replaced by integrals with the use of the equality

$$\sum_k \ldots = \frac{U_0 N}{k_{\parallel 0}^3 n} \int_0^{k_{\parallel 0}} \left(\int_0^{k'_\perp} \ldots k_\perp dk_\perp\right) \ldots dk_\parallel, \tag{1.36}$$

where $k'_\perp = \sqrt{s_2(k_{\parallel 0}^2 - k_\parallel^2)}$ and the limit values $k_{\parallel 0,\perp 0}$ are equal (n is the number of valleys)

$$k_{\parallel 0} = \left(\frac{3\pi^2 N}{vN_0 ns_2}\right)^{1/3}, \qquad s_2 = \frac{\bar{E}_4}{\bar{E}_2} = \left(\frac{k_{\perp 0}}{k_{\parallel 0}}\right)^2, \qquad U_0 = 3s_2^{-1} \tag{1.37}$$

with

$$\bar{E}_2 = \frac{\bar{E}_1}{4} + \gamma_{10}\sqrt{\frac{\Delta^2}{4} + \bar{E}_4}, \qquad \bar{E}_4 = \frac{\bar{E}_3}{4} + \frac{\gamma_{20}}{2}(\gamma_{20} + \sqrt{\Delta^2 + \gamma_{20}^2 + \bar{E}_3}). \tag{1.38}$$

385

and

$$\bar{E}_{1,3}=2\,(\bar{a}_{10,20}\Delta+2\bar{\mathcal{S}}^2_{\perp,\parallel}),\qquad \bar{a}_{10,20}=\bar{a}_{1,2}k^2_{\parallel 0}, \tag{1.39}$$

$$\gamma_{10,20}=\frac{\hbar^2}{2}M^-_{\perp,\parallel}k^2_{\parallel 0},\qquad \bar{\mathcal{S}}^2_{\perp,\parallel}=P^2_{\perp,\parallel}k^2_{\parallel 0}. \tag{1.40}$$

Then the squared soft-mode frequency in the paraphase is expressed as

$$M\Omega^2_{hs}=a_1=M\hat{\omega}^2_0-\frac{8}{3}\,[\bar{V}^2_\perp\,(2i_1-\bar{\mathcal{S}}^2_\perp\,i_{1\perp})+\bar{V}^2_\parallel\,(i_1-\bar{\mathcal{S}}^2_\parallel i_{1\parallel})], \tag{1.41}$$

where the quantity i_1, determining essentially the occurrence of the ferroelectric dynamic lattice instability, equals

$$i_1=\frac{U_0\varepsilon_0}{2}\,(C_0-\tau_1\varkappa^{-1}), \tag{1.42}$$

whereas

$$\varepsilon_0=\bar{E}^{-1/2}_1,\qquad C_0=C_{1,2}\delta_{1,2},\qquad C_{1,2}=\sqrt{\pm s_1\mp s_2}, \tag{1.43}$$

and

$$s_1=\frac{\bar{E}_3}{\bar{E}_1},\qquad \hat{\delta}_{1,2}=\delta_{1,2}+(\delta^2_{1,2}\mp1)L^{(1,2)}_1,\qquad \varkappa=s^{-1/2}_1, \tag{1.44}$$

$$\delta_{1,2}=\sqrt{\left(\frac{\Lambda}{C_{1,2}}\right)^2\pm1},\qquad \Lambda^2=s_2+\Delta^2\bar{E}^{-1}_1, \tag{1.45}$$

$$L^{(1)}_1=\mathrm{Arcth}\,\delta_1;\qquad L^{(2)}_1=\arcsin\,(\delta^2_2+1)^{-1/2}, \tag{1.46}$$

$$\delta_3=\sqrt{1+\Delta^2\bar{E}^{-1}_3},\qquad L_2=\mathrm{Arcth}\,\delta_3, \tag{1.47}$$

$$\tau_1=\delta_3+(\delta^2_3-1)L_2,\qquad \bar{V}_{\perp,\parallel}=V_{\perp,\parallel}\sqrt{\frac{N}{N_0n}}. \tag{1.48}$$

The quantities $i_{1\parallel,1\perp}$ determining essentially the stabilizing contribution to the soft-mode frequency Ω_{hs}, are equal to

$$i_{1\parallel}=\frac{U_0\varepsilon^3_0}{2}\,(D_2+\varkappa L_4),\qquad i_{1\perp}=\frac{U_0\varepsilon^3_0}{2}\left(\frac{2i_1}{U_0\varepsilon_0}+D_1-\frac{\tau_1}{\varkappa}\right) \tag{1.49}$$

with

$$L_4=2\delta_3-\tau_1,\qquad D_2=-C^{-1}_{1,2}L_3, \tag{1.50}$$

$$L_3=\pm2\delta_{1,2}\mp\hat{\delta}_{1,2},\qquad D_1=C^{-1}_{1,2}[\varkappa^{-2}L_3+2(\Lambda^2-s_2)L^{(1,2)}_1]. \tag{1.51}$$

Here C_1, δ_1, $L^{(1)}_1$, and upper signs correspond to $s_1>s_2$ and the lower ones and C_2, δ_2; $L^{(2)}_1$, to $s_1<s_2$. For $s_1=s_2$ ($\gamma_{10,20}=0$) in (1.42)—(1.51) we have

$$C_0=2\Lambda,\qquad D_1=\frac{2}{\Lambda}\left(\frac{1}{3\varkappa^2}+\frac{\Delta^2}{\bar{E}_1}\right),\qquad D_2=-\frac{2}{3\Lambda}. \tag{1.52}$$

From equations (1.41)—(1.52) it can be seen that the frequency of the FE vibration essentially depends on the details of the electronic band structure of $A^{IV}B^{VI}$-type compounds. The coefficients of the vibronic anharmonicity are calculated in Part 2, where a comparison with the experiment is also made.

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AⁱⱽBⱽⁱ ÜHENDITES ELEKTRON—FOONON-INTERAKTSIOONI POOLT INDUTSEERITUD SENJETTELEKTRILISTE FAASISIIRETE MIKROTEOORIA. 1

On arendatud AⁱⱽBⱽⁱ ühendites elektron—foonon-interaktsiooni poolt põhjustatud senjettelektriliste faasisiirete mikroteooria, võttes arvesse nende ainete reaalset tsoonistruktuuri. On arvutatud AⁱⱽBⱽⁱ senjettelektrikute-pooljuhtide vaba energia. Elektron—foonon-interaktsioon genereerib üheaegselt pehme võnkumise ja temperatuurist sõltuvad elastsus- ja elektrilise striktsiooni konstandid.

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МИКРОСКОПИЧЕСКАЯ ТЕОРИЯ СЕГНЕТОЭЛЕКТРИЧЕСКИХ ФАЗОВЫХ ПЕРЕХОДОВ, ИНДУЦИРОВАННЫХ ЭЛЕКТРОН-ФОНОННЫМ ВЗАИМОДЕЙСТВИЕМ В СОЕДИНЕНИЯХ AⁱⱽBⱽⁱ. 1

Развита микроскопическая теория сегнетоэлектрических фазовых переходов, обусловленных электрон-фононным взаимодействием в полупроводниках AⁱⱽBⱽⁱ, с учетом реальной электронной зонной структуры этих соединений. Получена свободная энергия сегнетоэлектриков-полупроводников AⁱⱽBⱽⁱ. Электрон-фононное взаимодействие одновременно генерирует мягкую моду и температурно зависящие упругие и электрострикционные постоянные.