SOLIDS

COMPLEX INTERFACE BETWEEN TWO MONOCLINIC PHASES

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A model of complex phase boundary, which includes an induced intermediate phase, is suggested. It has been shown that, provided the crystallographic parameters of two monoclinic phases do not satisfy the condition of thin interface formation, a complex phase interface characterized by two structures is formed. The minima in the temperature dependences of elastic energy of those two possible structures in the induced phase have been shown to correspond to the temperatures and the temperature hysteresis of a real phase transition, with $Pb_3(VO_4)_2$ being selected as an example.

1. Introduction

Provided that the phase transition is of the first kind, the mechanism of new phase formation governs the relative orientation of two phases and the habit of the interface between them [1, 2]. The majority of theoretical developments consider the phase interface as coherent, i.e. as a continuous transformation of a crystalline lattice into another one at the phase transition [3,4]. This means that lattice distortions have to match at the interface (i.e. the phase interface is considered as a plane, where distortions are absent [5]). Phenomenological models [6–8] were proposed to determine the orientation of the zero-distortion plane, provided that there is twinning at the interface. The calculated orientations of such interfaces agree well with experimental results for some phase transitions, but those models are incapable of determining the structure and orientation in a specific orientational state.

In work [9], the model of thin plane interface (TPI) – i.e. a direct contact – between two monoclinic phases was proposed, and, in works [10, 11], the

conditions for a TPI to be formed between phases with different symmetries were analyzed. For a TPI to emerge, certain relationships between variations of crystallographic parameters at a phase transition are to be satisfied. In addition, the crystallographic axes in one phase have to be rotated with respect to those in another phase; this rotation is associated with the Gibbs vector $\mathbf{G}_{fi}$.

In work [12], the temperature dependences of crystallographic parameters measured in two phases of pure ferroelastic $Pb_3(PO_4)_2$ were used to analyze the conditions of TPI formation at different temperatures. The energy density W of elastic lattice deformations at the phase transition and the density of the quantity $|\Delta G| = |G_i - G_{fi}|$, which characterizes the degree of orientational phase conformity at the TPI formation, were determined for each phase. Here, the Gibbs vector $\mathbf{G}_i$ corresponds to a spontaneous rotation of the ferroelastic phase with respect to the paraelastic one. It was also demonstrated that, in the range of the actual phase transition, there are minima in the temperature dependences of W and $|\Delta G|$.

The following issue remains obscured: Which are the structure and the orientation of phase interface, provided that the parameters of crystallographic lattices do not satisfy the condition of TPI formation at the phase transition. For this case, we have proposed a model of complex phase interface (CPI) with the induced phase as a component (Fig. 1). The induced phase puts distortions that emerge in two phases at the phase transition into agreement with the help of two parallel TPIs.

2. Complex Phase Interface Between Two Monoclinic Phases

Let us denote the crystallographic parameters of the first phase (β-phase) as a_1, b_1, c_1, β_1, and $\varphi_1 = \beta_1 - 90°$; the parameters of the induced phase as a_2, b_2, c_2, β_2, and $\varphi_2 = \beta_2 - 90°$; and the parameters of the second phase (α-phase) as a_3, b_3, c_3, β_3 and $\varphi_3 = \beta_3 - 90°$. The corresponding coordinate systems are (X_1, Y_1, Z_1), (X_2, Y_2, Z_2), and (X_3, Y_3, Z_3), where the X_i-axis is parallel to the c_i-axis, the Y_i-axis is parallel to the b_i-axis, and the Z_i-axis forms the angle φ_i with the a_i-axis (Fig. 1). The parameters α and β do not satisfy the condition of TPI formation at the phase transition.

Since the induced phase matches with the α- and β-phases by means of two parallel TPIs, its parameters must obey the equations for those TPIs. The equation for the TPI between the β- and induced phases (TPI$_1$) looks like

$$X_2^2 B_{11} + Y_2^2 B_{22} + Z_2^2 B_{33} + 2X_2 Z_2 B_{13} = 0 \qquad (1)$$

in the coordinate system of the second phase [10], where

$$B_{11} = 1 - (c_1/c_2)^2; \quad B_{22} = 1 - (b_1/b_2)^2;$$

$$B_{13} = -\frac{c_1}{c_2 \cos \varphi_2}\left(\frac{c_1}{c_2}\sin\varphi_2 - \frac{a_1}{a_2}\sin\varphi_1\right);$$

$$B_{33} = 1 - \frac{1}{\cos^2 \varphi_2}\left(\left(\frac{a_1}{a_2}\right)^2 \cos^2 \varphi_1 + \right.$$

$$\left. + \left(\frac{c_1}{c_2}\sin\varphi_2 - \frac{a_1}{a_2}\sin\varphi_1\right)^2\right).$$

If

$$B_{11}B_{33} - B_{13}^2 = 0, \quad B_{22}B_{11} \quad < \quad 0, \qquad (2)$$

Eq. (1) is equivalent to the following equations for two TPIs:

$$X_2 + B_2 Y_2 + K_2 Z_2 = 0, \qquad (3)$$

$$X_2 - B_2 Y_2 + K_2 Z_2 = 0, \qquad (4)$$

where $B_2 = \sqrt{-B_{22}/B_{11}}$ and $K_2 = B_{13}/B_{11}$.

In turn, the equation for the TPI between the α- and induced phases (TPI$_2$) looks like

$$X_2^2 C_{11} + Y_2^2 C_{22} + Z_2^2 C_{33} + 2X_2 Z_2 C_{13} = 0,$$
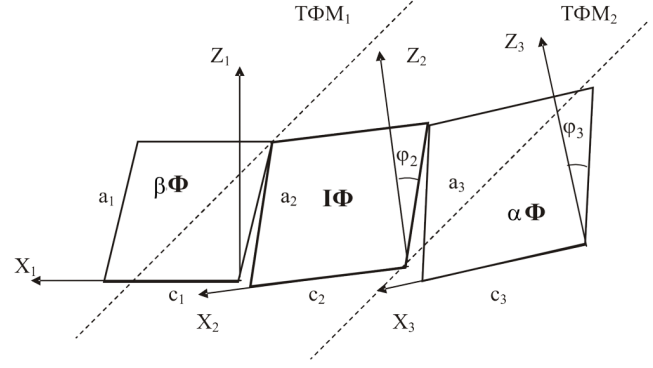

Fig. 1. Structure of a complex phase interface

where

$$C_{11} = 1 - (c_3/c_2)^2; \quad C_{22} = 1 - (b_3/b_2)^2;$$

$$C_{13} = -\frac{c_3}{c_2 \cos \varphi_2}\left(\frac{c_3}{c_2}\sin\varphi_2 - \frac{a_3}{a_2}\sin\varphi_3\right);$$

$$C_{33} = 1 - \frac{1}{\cos^2 \varphi_2}\left(\left(\frac{a_3}{a_2}\right)^2 \cos^2 \varphi_3 + \right.$$

$$\left. + \left(\frac{c_3}{c_2}\sin\varphi_2 - \frac{a_3}{a_2}\sin\varphi_3\right)^2\right).$$

Provided

$$C_{11}C_{33} - C_{13}^2 = 0, \quad C_{22}C_{11} \quad < \quad 0, \qquad (5)$$

Eq. (1) also corresponds to the equations for two TPIs,

$$X_2 + B_3 Y_2 + K_3 Z_2 = 0, \qquad (6)$$

$$X_2 - B_3 Y_2 + K_3 Z_2 = 0, \qquad (7)$$

where

$$B_3 = \sqrt{-C_{22}/C_{11}}, \quad K_3 = C_{13}/C_{11}.$$

Hence, two CPI orientations (CPI$_1$ and CPI$_2$) are possible. They are associated with Eqs. (3), (6) and (4), (7), respectively.

Consider the structure of CPI$_1$. Since TPI$_1$ and TPI$_2$ are parallel to each other, we obtain from Eqs. (3) and (6) that

$$B_2 = B_3, \quad K_2 = K_3. \qquad (8)$$

From Eqs. (2), (5), and (8), we compose a system, consisting of four equations and two inequalities, to determine four unknown parameters for the induced phase:

$$
\begin{cases}
B_2 = B_3, \\
K_2 = K_3, \\
B_{11}B_{33} - B_{13}^2 = 0, \\
C_{11}C_{33} - C_{13}^2 = 0, \\
B_{22}B_{11} \triangleleft 0, \\
C_{22}C_{11} \triangleleft 0.
\end{cases}
\tag{9}
$$

The solutions of system (9) are

$$
c_2 = \sqrt{\frac{-B \pm \sqrt{B^2 - 4HM}}{2H}};
$$

$$
b_2 = \sqrt{\frac{c_2^2(b_3^2 - b_1^2) + b_1^2 c_3^2 - b_3^2 c_1^2}{c_3^2 - c_1^2}};
$$

$$
\varphi_2 = \operatorname{arctg}(F/\sqrt{Q}); \quad a_2 = F/\sin(\varphi_2), \tag{10}
$$

where

$$
H = a_1^2 - a_3^2 + m^2/(c_3^2 - c_1^2);
$$

$$
M = n^2(f - p) + n(hc_3^2 - qc_1^2) + kc_3^2 - Lc_1^2;
$$

$$
B = c_3^2 \cos^2(\varphi_3)a_3^2 - c_1^2 \cos^2(\varphi_1)a_1^2 +
$$

$$
+ c_1^2 a_3^2 - a_1^2 c_3^2 + 2mn/(c_3^2 - c_1^2);
$$

$$
Q = \left(c_2^4 a_1^2 + (c_2^2 m + n)^2 f - \right.
$$

$$
- (c_2^4 m + c_2^2 n)h - c_2^2 k)/(c_2^2(c_2^2 - c_1^2));
$$

$$
f = c_1^2/(c_3^2 - c_1^2)^2; \quad F = (c_2^2 m + n)/(c_2(c_3^2 - c_1^2));
$$

$$
m = c_3 a_3 \sin(\varphi_3) - c_1 a_1 \sin(\varphi_1);
$$

$$
n = c_1 a_1 c_3^2 \sin(\varphi_1) - c_3 a_3 c_1^2 \sin(\varphi_3);
$$

$$
h = 2c_1 a_1 \sin(\varphi_1)/(c_3^2 - c_1^2);
$$

$$
k = (c_1 \cos(\varphi_1)a_1)^2; \quad p = c_3^2/(c_3^2 - c_1^2)^2;
$$

$$
q = 2c_3 a_3 \sin(\varphi_3)/(c_3^2 - c_1^2); \quad L = (c_3 \cos(\varphi_3)a_3)^2.
$$

The c_2-parameter can acquire two values,

$$
c_2 = \sqrt{\frac{-B + \sqrt{B^2 - 4HM}}{2H}};
$$

$$
c_2 = \sqrt{\frac{-B - \sqrt{B^2 - 4HM}}{2H}}.
$$

Therefore, two structures in the induced phase are possible (A and B, respectively). Since the change of sign of coefficients B_2 and B_3 does not affect the solution of system (9), the structure of CPI$_2$ is similar to that of CPI$_1$.

The parameters of the induced phase are known. Hence, it is possible to obtain the equations for CPI$_1$ and CPI$_2$ in the coordinate systems of the α- and β-phases, respectively:

$$
X_1 + B_1 Y_1 + K_1 Z_1 = 0, \tag{11}
$$

$$
X_1 - B_1 Y_1 + K_1 Z_1 = 0, \tag{12}
$$

$$
X_3 + B_4 Y_3 + K_4 Z_3 = 0, \tag{13}
$$

$$
X_3 - B_4 Y_3 + K_4 Z_3 = 0, \tag{14}
$$

where

$$
B_1 = \sqrt{-A_{22}/A_{11}}, \quad K_1 = A_{13}/A_{11},
$$

$$
B_4 = \sqrt{-D_{22}/D_{11}}, \quad K_4 = D_{13}/D_{11},
$$

$$
A_{11} = 1 - (c_2/c_1)^2; \quad A_{22} = 1 - (b_2/b_1)^2;
$$

$$
D_{11} = 1 - (c_2/c_3)^2; \quad D_{22} = 1 - (b_2/b_3)^2;
$$

$$
A_{13} = -\frac{c_2}{c_1 \cos \varphi_1}\left(\frac{c_2}{c_1}\sin \varphi_1 - \frac{a_2}{a_1}\sin \varphi_2\right);
$$

$$
D_{13} = -\frac{c_2}{c_3 \cos \varphi_3}\left(\frac{c_2}{c_3}\sin \varphi_3 - \frac{a_2}{a_3}\sin \varphi_2\right).
$$

Making use of Eqs. (11) and (13), we obtain the coordinates of the Gibbs vector $\mathbf{G}_{f1}$ which characterizes a rotation of the α-phase with respect to the β-one:

$$\mathbf{G}_{f1} = h_1\mathbf{e}_1 + h_2\mathbf{e}_2 + h_3\mathbf{e}_3, \qquad (15)$$

where

$$h_1 = r_1\,\mathrm{tg}(\delta_2/2);\quad h_2 = r_2\,\mathrm{tg}(\delta_2/2);\quad h_3 = r_3\,\mathrm{tg}(\delta_2/2);$$

$$r_1 = \frac{d_1}{|d|};\quad r_2 = \frac{d_2}{|d|};\quad r_3 = \frac{d_3}{|d|};\delta_2 = \arccos(S_2);$$

$$d_1 = B_1K_4 - B_4K_1;\quad d_2 = K_1 - K_4;$$

$$d_3 = B_4 - B_1;\quad |d| = \sqrt{d_1^2 + d_2^2 + d_3^2};$$

$$S_2 = \frac{1 + B_1B_4 + K_1K_4}{\sqrt{(1+B_1^2+K_1^2)(1+B_4^2+K_4^2)}}.$$

Equations (12) and (14) are used analogously to determine the vector $\mathbf{G}_{f2}$.

Hence, when the CPI is formed, the α-phase can be in either of two orientational positions, depending on which CPI (CPI$_1$ or CPI$_2$) is realized. Two vectors, $\mathbf{G}_{f1}$ and $\mathbf{G}_{f2}$, are associated with them. To elucidate which conditions are needed for either structure A or B to be realized in the induced phase, we will analyze the CPI structure in a pure ferroelastic Pb$_3$(VO$_4$)$_2$ which undergoes the $\gamma \to \beta$ phase transition of the first kind $\bar{3}mF2/m$ at a temperature of 360 K [13]. According to the notations introduced above when considering the CPI model, the γ-phase is adopted as the first one (pseudomonoclinic), and the β-phase as the second one (monoclinic). In this crystal, as was shown in work [14], the linear dependences of crystallographic parameters on the parameter c are observed within both phases. The following regression lines correspond to them: in the γ-phase,

$$a_1 = k_1c + d_1; b_1 = c/\sqrt{3};\quad \varphi_1 = k_2c + d_2; \qquad (16)$$

and, in the β-phase,

$$a_2 = k_3c + d_3; b_2 = k_4c + d_4;\quad \varphi_2 = k_5c + d_5; \qquad (17)$$

where
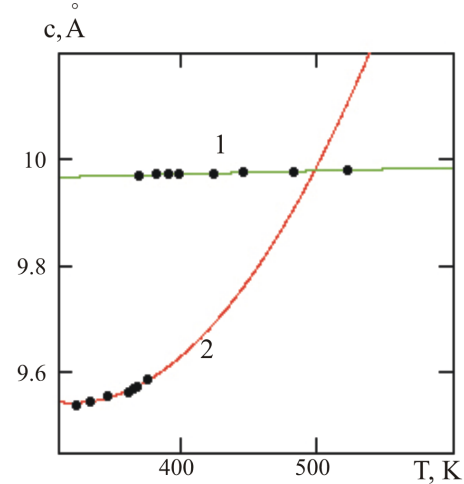
$$k_1 = 2.004;\quad d_1 = -12.42;\quad k_2 = -0.0889;$$

Fig. 2. Temperature dependence of the crystallographic parameter c in the γ-phase (1) and in the β-phase (2)

$$d_2 = 1.342;\quad k_3 = 0.408;\quad d_3 = 3.624;$$

$$k_4 = -0.688;\quad d_4 = 12.66;\quad k_5 = 0.039;\quad d_5 = 0.0675.$$

Near the phase transition point (in the range 320–371 K), the temperature dependence of the parameter c is linear in the γ- phase and can be approximated well by a square law in the β-phase (Fig. 2). The points in this figure correspond to experimental values, and curves to the following regression equations:

$$c_1 = k_6T + d_6; \qquad (18)$$

$$c_2 = k_7T^2 + k_8T + k_9, \qquad (19)$$

where

$$k_6 = 6.27 \times 10^{-5};\quad d_6 = 9.947;\quad k_7 = 1.379 \times 10^{-5};$$

$$k_8 = -0.0088;\quad k_9 = 10.95.$$

Substituting Eq. (18) into Eq. (16) and Eq. (19) into Eq. (17), we obtain the temperature dependences of the crystallographic parameters in both phases near the phase transition point. From Eqs. (10)–(14), we obtain the induced-phase parameters and the equations for CPI. This allows the temperature dependences of the elastic energy in the induced phase and the orientational phase conformity to be analyzed.

Two densities of elastic energy, W_A and W_B, correspond to two possible structures (A and B) of the induced phase in the CPI. They both are the sum of
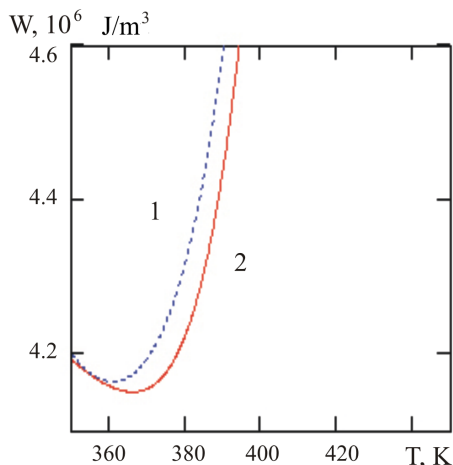
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W, 10^6 J/m³

Fig. 3. Temperature dependences of the elastic energy densities W_B (1) and W_A (2)

induced-phase deformation energies determined relatively to the parameters of the γ- and β-phases:

$$W_A = W_{A1} + W_{A2}; \quad W_{A1} = 0.5C_{ijkl}e_{A1ij}e_{A1kl};$$

$$W_{A2} = 0.5C_{ijkl}e_{A2ij}e_{A2kl}; \tag{20}$$

$$W_B = W_{B1} + W_{B2}; \quad W_{B1} = 0.5C_{ijkl}e_{B1ij}e_{B1kl};$$

$$W_{B2} = 0.5C_{ijkl}e_{B2ij}e_{B2kl}, \tag{21}$$

where C_{ijkl} are the moduli of elasticity [15, 16]; e_{A1ij} and e_{B1ij} are the strain tensors for the induced phase, which correspond to structures A and B, respectively, relatively to the γ-phase parameters; and e_{A2ij} and e_{B2ij}

are the strain tensors of those two structures relative to the β-phase.

Figure 3 demonstrates the temperature dependences of W_A and W_B. There are the minima in the elastic energy densities at T_A and T_B, with the W_A-minimum being shifted with respect to the W_B-minimum by $\Delta T = 7.6$ K toward higher temperatures. The locations of those minima agree well with the actual temperatures of the $\gamma \to \beta$ and $\beta \to \gamma$ phase transitions (see Table). The induced phase has monoclinic symmetry, with the crystallographic parameters of structure A being closer to the corresponding parameters of the γ-phase, while those of structure B to the parameters of the β-phase. Hence, structure B of induced phase in CPI is formed at the $\gamma \to \beta$ phase transitions, and structure A at the $\beta \to \gamma$ ones.

Structure A in the induced phase at T_A is associated with two CPI equations in the coordinate system of the γ-phase:

$$X_1 \pm 1.207Y_1 + 0.052Z_1 = 0. \tag{22}$$

The angles between the traces of two CPIs on the (001) plane, on the one hand, and the b_1-axis, on the other hand, are $\alpha = \pm 50.36°$, which agrees well with the experimental results $\alpha = \pm(50\pm1)°$ [17]. For the case of the structure B formation at T_B, the CPI equations are almost identical to Eqs. (22) (the orientation difference is about 0.002°).

For this kind of phase transition, the coordinates of the Gibbs vector $\mathbf{G}_i$, which characterizes a spontaneous rotation of the ferroelastic phase with respect to the paraelastic one, were determined in work [18] as

$$\mathbf{G}_i = g_1\mathbf{e}_1 + g_2\mathbf{e}_2 + g_3\mathbf{e}_3, \tag{23}$$

Phase transition temperatures and phase parameters for Pb₃(VO₄)₂

Parameter	Calculation		Experiment [13]	
	$\beta \to \gamma$ (structure A)	$\gamma \to \beta$ (structure B)	$\beta \to \gamma$	$\gamma \to \beta$
a_1,Å	7.555	7.554	7.555	7.548
b_1,Å	5.756	5.756	5.757	5.759
c_1,Å	9.97	9.9696	9.969	9.962
β_1,°	116.09	116.095	116.09	116.16
a_2,Å	$7.555 + 2.4 \times 10^{-2}$	$7.53 - 2.3 \times 10^{-2}$	–	–
b_2,Å	$5.756 + 4.6 \times 10^{-12}$	$6.079 - 2.7 \times 10^{-12}$	–	–
c_2,Å	$9.97 - 5.4 \times 10^{-12}$	$9.566 + 3.5 \times 10^{-12}$	–	–
β_2,°	$116.09 - 8.9 \times 10^{-2}$	$115.28 + 8.3 \times 10^{-2}$	–	–
a_3,Å	7.535	7.53	7.531	7.53
b_3,Å	6.073	6.079	6.065	6.075
c_3,Å	9.575	9.566	9.583	9.573
β_3,°	115.3	115.28	115.39	115.3
T_i, K	365.94	358.34	368	360

where

$$g_1 = \frac{e_1 \operatorname{tg}(\delta/2)}{M}; \quad g_2 = \frac{e_2 \operatorname{tg}(\delta/2)}{M}; \quad g_3 = \frac{e_3 \operatorname{tg}(\delta/2)}{M};$$

$$e_1 = \sqrt{3}K_7 - B_7 K_6; \quad e_2 = K_6 - K_7; \quad e_3 = B_7 - \sqrt{3};$$

$$M = \sqrt{e_1^2 + e_2^2 + e_3^2};$$

$$\delta = \arccos(\frac{1 + \sqrt{3}B_7 + K_6 K_7}{\sqrt{(4 + K_6^2)(1 + B_7^2 + K_7^2)}});$$

$$K_6 = -2e_{13}^s / e_{11}^s; \quad K_7 = -\frac{2e_{13}^s(1 - e_{11}^s/2)}{e_{11}^s + 2e_{13}^{s\,2}},$$

$$B_7 = \frac{\sqrt{3}e_{11}^s(1 - e_{11}^s - e_{13}^{s\,2})}{(1 + e_{11}^s)(e_{11}^s + 2e_{13}^{s\,2})}.$$

Making use of Eqs. (15) and (23), we can determine the temperature dependences for $|\Delta G_A|$ and $|\Delta G_B|$. These two quantities describe the orientational conformity of the γ- and β-phases on the formation of two structures in CPI:

$$|\Delta G_A| = |G_{f1A} - G_1|, \quad |\Delta G_B| = |G_{f1B} - G_1|. \quad (24)$$

Here, $\mathbf{G}_{f1A}$ and $\mathbf{G}_{f1B}$ are the Gibbs vectors that characterize a rotation of the coordinate system of the β-phase with respect to the γ-phase on the formation of CPI, provided that the latter includes the induced phase with structure A or B, respectively; and $\mathbf{G}_1$ is the Gibbs vector that corresponds to a spontaneous rotation of the β-phase with respect to the γ-phase at the phase transition temperature.

Figure 4 illustrates the temperature dependences of $|\Delta G_A|$ and $|\Delta G_B|$. The curves almost coincide (the temperature shift is about 0.4 K). Hence, those absolute values have minima at temperatures that are much higher than the phase transition temperature (T_c). In particular, at $T = T_c$, we have $|\Delta G_A| \approx |\Delta G_B| = 3.55 \times 10^{-3}$, which is by an order of magnitude larger than the corresponding value obtained on the formation of TPI in $Pb_3(PO_4)_2$ [12]. Hence, the formation of CPI in $Pb_3(PO_4)_2$ is accompanied by a significant orientational mismatch between the phases, and this circumstance is most likely a key reason why a fine domain structure is formed, and why cracks are formed on the phase transition.

Thus, the analysis of the CPI structure in $Pb_3(PO_4)_2$ carried out in the framework of the model proposed makes it possible to draw a conclusion that the parameters of a phase induced in CPI correspond to two structures. The specific collection of parameters depends on the direction of the phase transition (direct or
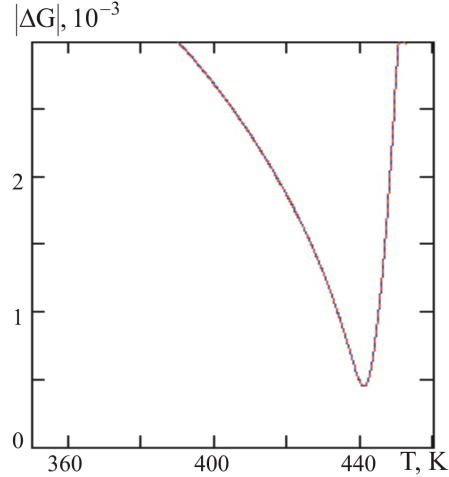

Fig. 4. Temperature dependences of $|\Delta G_A|$ and $|\Delta G_B|$

inverse), being closer to the corresponding parameters in either phase. The phase transition occurs at a temperature, at which the elastic energy of the corresponding structure in the induced phase is minimal. On the CPI formation, there emerges a certain orientational mismatch between the phases which is responsible for the polydomain state of ferroelastic crystals.

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СКЛАДНА ФАЗОВА МЕЖА МІЖ ДВОМА
МОНОКЛІННИМИ ФАЗАМИ

В.А. Непочатенко

Р е з ю м е

Запропоновано модель складної фазової межі, яка включає індуковану проміжну фазу. Показано, що у випадку, коли кристалографічні параметри двох моноклінних фаз не задовольняють умову формування тонкої фазової межі, утворюється складна фазова межа, яка може мати дві структури. На прикладі фазового переходу в $Pb_3(VO_4)_2$ показано, що мінімуми температурних залежностей пружних енергій двох можливих структур індукованої фази відповідні температурам і температурному гістерезису реального фазового переходу.