THIN INTERFACES BETWEEN TRICLINIC PHASES

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A model of the thin planar interface between triclinic phases is proposed, and the equations and conditions defining its formation are presented. It is shown that from one to four interfaces with different orientations can be formed depending on a variation of the parameters at a phase transition. The connection between the numbers of possible interfaces and suborientational states (SOS) is established.

1. Introduction

For the first time, the definition of the orientation of interfaces for some martensitic phase transitions was given in works [1—4]. There, it was shown that, in the case where a structural deformation is characterized by the invariant plane, the interface is a crystallographic plane without a layer where the phases would elastically coexist. In other cases, the interface is in a stressed state. As for the orientation of interfaces, their determination, according to the theory, is a quite complicated task solved only for some phase transitions [5,6].

In work [7], a model of the thin planar interface (TPI) (under a direct contact of two phases) adjusting two monoclinic phases was proposed. According to the model, an unstressed planar interface must not necessarily be a crystallographic plane. For the formation of TPI, the certain relations between variations in the parameters of phases at a first-order phase transition should be fulfilled. It was shown that two TPI can be formed in the general case. Upon the creation of such an interface, the lattices of two phases turn by a small angle. Moreover, the orientations of the rotation axes and the angle signs are different for two possible TPI, which leads to the formation of two close orientational states (suborientational ones) [8].

The determination of the number of possible SOS is a separate problem in the theory of polymorphic phase transitions. The equations defining TPI are also used in the determination of a structure of Seignette-elastic domain walls [9,10]. But the equations for TPI cannot be deduced from the analysis of results in the case where one (or both) phase is triclinic [7].

Thus, it is of interest to find the equations for TPI and the number of possible SOS upon a first-order phase transition between triclinic phases.

We choose the following orthogonal coordinate system: the a axis is parallel to the X_1 axis, the b axis is in the plane X_1OX_2 and forms an angle $\varphi = \gamma - 90°$ with X_2, the c axis forms an angle ψ with X_3, and the projection of the c axis on the plane X_1OX_2 forms an angle ω with X_1 (see the figure). The angles ψ and ω are defined by the equations

$$\omega = \mathrm{arctg}(\mathrm{ctg}\,\gamma + \cos\alpha/(\cos\beta\sin\gamma)), \tag{1}$$

$$\psi = \arcsin(\cos\beta/\cos\omega), \tag{2}$$

where α, β, γ are the angles between the corresponding axes.

We denote the parameters of the first phase as $a_1, b_1, c_1, \alpha_1, \beta_1, \gamma_1$ and those of the second one as $a_2, b_2, c_2, \alpha_2, \beta_2, \gamma_2$. The relevant crystallophysical axes are X_{i1}, X_{i2}.

2. The Equations for a Thin Interface between Triclinic Phases

We assume that, upon the formation of TPI, all the points of the interface are common for two different crystal lattices. This means that if we set the coordinate origin on the interface, the corresponding indices and the modulus of the radius vector for any site on the interface are the same relative to both lattices. The radius vector $\mathbf{r}_1$ which joins the coordinate origin and a site of the lattice of the first phase can be presented as (figure, a)

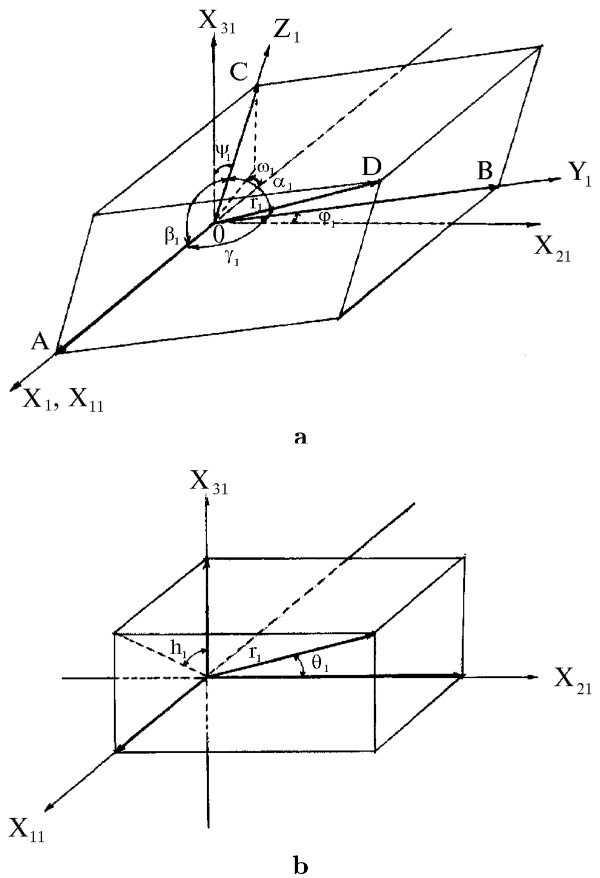
$$\mathbf{r}_1 = \mathbf{OD} = \mathbf{OA} + \mathbf{OB} + \mathbf{OC} = n_1\mathbf{a}_1 + m_1\mathbf{b}_1 + k_1\mathbf{c}_1, \tag{3}$$

where n_1, m_1, and k_1 are the site indices.

In the orthogonal coordinate system, coordinates $\mathbf{r}_1$ are (figure, b)

$$r_{x1} = r_1\sin\theta_1\sin\eta_1, \quad r_{x2} = r_1\cos\theta_1,$$

$$r_{x3} = r_1\sin\theta_1\cos\eta_1. \tag{4}$$



Definition of the radius-vector $\mathbf{r}_1$ in the crystallographic (a) and crystallophysical (b) coordinate systems

The corresponding coordinates $\mathbf{r}_1$ in the crystallographic coordinate system are as follows:

$$OA = r_1 M_1, \tag{5}$$

$$OB = r_1 N_1, \tag{6}$$

$$OC = r_1 K_1, \tag{7}$$

where $M_1 = \cos\theta_1 \mathrm{tg}\varphi_1 + \sin\theta_1(\sin\eta_1 + \cos\eta_1\ \mathrm{tg}\psi_1\ (\cos\omega_1 + \sin\omega_1\ \mathrm{tg}\varphi_1))$, $N_1 = (\cos\theta_1 + \sin\theta_1\ \cos\eta_1\ \mathrm{tg}\psi_1\ \sin\omega_1)/\cos\varphi_1$, $K_1 = \sin\theta_1\ \cos\eta_1/\cos\psi_1$.

Relations (3)—(7) yield

$$r_1 = \frac{n_1 a_1}{M_1} = \frac{m_1 b_1}{N_1} = \frac{k_1 c_1}{K_1}. \tag{8}$$

Analogously, we get the equations for the radius vector $\mathbf{r}_2$ which indicates a common site of the interface in the coordinate system of the second phase:

$$r_2 = \frac{n_2 a_2}{M_2} = \frac{m_2 b_2}{N_2} = \frac{k_2 c_2}{K_2}, \tag{9}$$

where $M_2 = \cos\theta_2 \mathrm{tg}\varphi_2 + \sin\theta_2\ (\ \sin\eta_2 + \cos\eta_2\ \mathrm{tg}\psi_2\ (\cos\omega_2 + \sin\omega_2\ \mathrm{tg}\varphi_2))$, $N_2 = (\cos\theta_2 + \sin\theta_2\ \cos\eta_2\ \mathrm{tg}\psi_2\ \sin\omega_2)/\cos\varphi_2$, $K_2 = \sin\theta_2\ \cos\eta_2/\cos\psi_2$.

According to the above-presented condition imposed on TPI, we obtain

$$r_1 = r_2, \quad n_1 = n_2, \quad m_1 = m_2, \quad k_1 = k_2. \tag{10}$$

From (8)—(10), we get the system

$$\begin{cases} a_1/M_1 = a_2/M_2, \\ b_1/N_1 = b_2/N_2, \\ c_1/K_1 = c_2/K_2. \end{cases} \tag{11}$$

The system of equations (11) can be solved in the coordinate systems of the first and second phases. In view of the relation

$$r_1^2 = x_{i1}^2, \tag{12}$$

we obtain the following equation in the coordinate system of the first phase:

$$X_{11}^2 A_{11} + X_{21}^2 A_{22} + X_{31}^2 A_{33} + 2X_{11}X_{21}A_{12} +$$

$$+ 2X_{11}X_{31}A_{13} + 2X_{21}X_{31}A_{23} = 0, \tag{13}$$

where $A_{11} = 1 - (a_2/a_1)^2$, $A_{22} = 1 - m^2 - H^2$, $A_{33} = 1 - n^2 - p^2 - G^2$, $A_{12} = -Ha_2/a_1$, $A_{13} = -Ga_2/a_1, A_{23} = -(mn + HG), m = b_2\cos\varphi_2/(b_1\cos\varphi_1)$, $p = c_2\cos\psi_2/(c_1\cos\psi_1)$, $n = m\mathrm{tg}\psi_1\sin\omega_1 - p\mathrm{tg}\psi_2\sin\omega_2$, $H = a_2\mathrm{tg}\varphi_1/a_1 - m\mathrm{tg}\varphi_2$, $G = a_2\mathrm{tg}\psi_1(\cos\omega_1 + \sin\omega_1\mathrm{tg}\varphi_1)/a_1 - n\mathrm{tg}\varphi_2 - p\mathrm{tg}\psi_2(\cos\omega_2 + \sin\omega_2\mathrm{tg}\varphi_2)$.

If $A_{11} \neq 0$, then relations (13) under the condition

$$\det|A_{ij}| = 0, \tag{14}$$

$$D_{12}^2 - D_{22} > 0, \quad D_{13}^2 - D_{33} > 0, \tag{15}$$

where $D_{ij} = A_{ij}/A_{11}$,
correspond to two pairs of equations for the intersecting planes (four TPI):

$$X_{11} + B_1 X_{21} + C_1 X_{31} = 0, \tag{16}$$

$$X_{11} + F_1 X_{21} + R_1 X_{31} = 0, \tag{17}$$

where $B_1 = D_{12} + \sqrt{D_{12}^2 - D_{22}}$; $F_1 = D_{12} - \sqrt{D_{12}^2 - D_{22}}$, $C_1 = D_{13} \pm \sqrt{D_{13}^2 - D_{33}}, R_1 = D_{13} \mp \sqrt{D_{13}^2 - D_{33}}$.

Solving analogously system (11) in the coordinate system of the second phase, we arrive at the equation

$$X_{12}^2 B_{11} + X_{22}^2 B_{22} + X_{32}^2 B_{33} + 2X_{12}X_{22}B_{12} +$$

$$+2X_{12}X_{32}B_{13} + 2X_{22}X_{32}B_{23} = 0, \quad (18)$$

where $B_{11} = 1 - (a_1/a_2)^2$, $B_{22} = 1 - 1/m^2 - L^2$, $B_{33} = 1 - k^2 - 1/p^2 - E^2$, $B_{12} = -La_1/a_2$, $B_{13} = -Ea_1/a_2$, $B_{23} = -(k/m + LE)$, $m = b_2 \cos\varphi_2/(b_1 \cos\varphi_1)$, $p = c_2 \cos\psi_2/(c_1 \cos\psi_1)$, $k = \mathrm{tg}\psi_2 \sin\omega_2/m - \mathrm{tg}\psi_1 \sin\omega_1/p$, $L = a_1\mathrm{tg}\varphi_2/a_2 - \mathrm{tg}\varphi_1/m$, $-E = a_1\mathrm{tg}\psi_2(\cos\omega_2 + \sin\omega_2\mathrm{tg}\varphi_2)/a_2 - k\mathrm{tg}\varphi_1 - \mathrm{tg}\psi_1(\cos\omega_1 + \sin\omega_1\mathrm{tg}\varphi_1)/p$.

If conditions (14) and (15) are satisfied, Eq. (18) corresponds also to two pairs of the equations for TPI:

$$X_{12} + B_2X_{22} + C_2X_{32} = 0, \quad (19)$$

$$X_{12} + F_2X_{22} + R_2X_{32} = 0, \quad (20)$$

where $B_2 = C_{12} + \sqrt{C_{12}^2 - C_{22}}$; $F_2 = C_{12} - \sqrt{C_{12}^2 - C_{22}}$, $C_2 = C_{13} \pm \sqrt{C_{13}^2 - C_{33}}$, $R_2 = C_{13} \mp \sqrt{C_{13}^2 - C_{33}}$, $C_{ij} = B_{ij}/B_{11}$.

If the equations for TPI relative to two coordinate systems are known, we may define the transformation matrices for the transition from the coordinate system of the first phase to that of the second one which correspond to a specific SOS [8]. Because each TPI forms a separate orientational state, four SOS are possible, which is twice more than those at a phase transition between monoclinic phases [8].

If one of the conditions

$$C_{12}^2 - C_{22} = 0, \quad (21)$$

$$C_{13}^2 - C_{33} = 0 \quad (22)$$

is satisfied, only two different TPI are formed, and, respectively, two SOS. We call this as the two-fold degeneracy of an interface. If (21) and (22) are valid, then we are faced with the three-fold degeneracy, and only one TPI is possible. In this case, SOS is absent.

If one of the coefficients $C_{ii} = 0$, an interface can be formed, whose normal is perpendicular to a crystallographic axis. If two coefficients are zero, then the normal is parallel to a crystallographic axis.

As known, two [8,11] or four [12] SOS are formed at polymorphic phase transitions between phases with a symmetry higher than the triclinic one. The nature of their formation is unclear, and the derived results of the analysis of TPI testify to that they can be conditioned by aspects not related to a symmetry.

Thus, it follows from the proposed model of thin interfaces that one, two, or four thin interfaces different by their orientations can be created at the first-order phase transition between triclinic phases. Each interface forms a certain orientational state, the number of suborientational states can be only an even value, and their existence does not related to the presence of any symmetry elements.

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ТОНКІ ФАЗОВІ МЕЖІ МІЖ ТРИКЛІННИМИ ФАЗАМИ

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Р е з ю м е

Запропоновано модель тонкої плоскої фазової межі між триклінними фазами. Визначено рівняння і умови її формування. Показано, що в залежності від зміни параметрів в околі фазового переходу можливе формування від однієї до чотирьох різних за орієнтацією фазових меж. Встановлено взаємозв'язок між кількістю можливих фазових меж і субoрієнтаційних станів.