

## THE GROWTH CHARACTERISTICS OF THE III–V COMPOUND-LIKE CRYSTALS AFFECTED BY THE RELATIVE ACTIVITY

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The growth characteristics of a stoichiometric compound crystal with tetrahedral bonding such as II–VI and III–V compound are considered. Just because of an asymmetric nature of bonding, the growth characteristics controlled by the surface kinetics need modifications as compared to the case of a crystal with symmetric bonding. The difference of growth behaviors in the positive direction from those in the negative direction along the polar axis is of special interest. The 2D nucleation on a singular surface and the step motion in a singular orientation are treated. It can be shown that the growth features under a given driving force,  $\Delta\mu = \Delta\mu_A + \Delta\mu_B$ , vary depending on the relative activity,  $\Delta\mu_A - \Delta\mu_B$ , of the constituent components in the environment. Any effect due to the difference of chemical nature of constituent elements as well as to specific complex as in the case of CVD method is neglected.

### 1. 2D Nucleation

The Wulff's theorem determining the optimum form of nucleus can be extended to predict the optimum form and size of nucleus by taking account of the supersaturated environment.

$$\Delta G_A = -(\Delta\mu_A N_A + \Delta\mu_B N_B) + \frac{\phi}{2}(N_A - N_B) + \sum \gamma_c(\vec{n}_i) l_i \rightarrow \text{optimum} .$$

In the case of layer by layer thickening of a singular surface, (111) of the zinc blend type crystal and (0001) of the wurzite type crystal, 2D island is constituted of double layer, one A-layer and one B-layer. The contributions of the  $\langle \bar{1}11 \rangle$ ,  $\langle 1\bar{1}1 \rangle$  and  $\langle 11\bar{1} \rangle$  bonding to the step energy  $\gamma(\vec{n})$  is obtained by the

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bond breaking method according to  $\gamma(\vec{n})=\gamma(-\vec{n})=(1/2)$  [cutting energy]. The obtained polar graph  $\gamma(\vec{n})$  is very much scattered as compared to the case of symmetric bonding, because of the dependence of the cutting energy for given  $\vec{n}$  on the exact position of the cut plane. The contribution of the  $\langle 111 \rangle$  bonding normal to the singular substrate is favorable for B-atoms and unfavorable for A-atoms on an A-face. This circumstance gives rise to the difference of the optimum form and size of the 2D nucleus and accordingly of the energy of nucleation  $\Delta G^*$ , whether it is on the positive (111) A-face or on the negative ( $\bar{1}\bar{1}\bar{1}$ ) B-face. It is notable that the optimum form of the nucleus is not definite just related to the polar graph  $\gamma(\vec{n})$  but varies according to the relative activity,  $\Delta\mu_A - \Delta\mu_B$ . It can be concluded that, provided  $\Delta\mu_A > \Delta\mu_B$ , 2D nucleation on an A-face is more favorable than on B-face,  $\Delta G_A^* < \Delta G_B^*$ , and vice versa.

## 2. Step Motion

The growth of the double layer initiated on the singular surface (111) by 2D nucleation or screw mechanism is finally controlled by the advancement of singular steps, each in directions  $\langle 11\bar{2} \rangle$ ,  $\langle 1\bar{2}1 \rangle$  and  $\langle \bar{2}11 \rangle$ . As to the arrangement of atoms at a kink on these singular steps, two kinds of kink states are discriminated, a kink state  $k_A$  occupied by an A-atom and a kink state  $k_B$  occupied by a B-atom. The kink energies of  $k_A$  and  $k_B$  is approximately the same, but the way of transport of respective atoms is quite different. In the case of (111) A-face, while the transport of A-atom to the  $k_A$ -site is furnished just by direct flight from the vapor, the transport of B-atom to the  $k_B$ -site is enhanced through the contribution of surface migration of B-adatoms on the A-face. The net flows  $J_A$  and  $J_B$  of respective atoms under situation ( $p_A, p_B$ ) can be written as

$$J_A = N_B \frac{a^2}{\sqrt{2\pi m_A k T}} (p_A - p_{A0}), \quad J_B = N_A \frac{x_B^2}{\sqrt{2\pi m_B k T}} (p_B - p_{B0}),$$

where the reference state ( $p_{A0}, p_{B0}$ ) is to be determined to give the steady kink structure ( $N_A, N_B$ ). If  $x_B \gg a$ , it can be shown that, under steady condition ( $J_A = J_B$ ) on a A-face, the distribution of component B is nearly stagnant ( $p_{B0} \approx p_B$ ) and the advancement of the step is controlled just by the activity of component A.