Spinodal decomposition ranges of $In_x\,Ga_{1-x}\,N_y\,P_{1-y}$
and $GaAs_x\,N_y\,P_{1-x-y}$ alloys

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We have described spinodal decomposition ranges of GaP-rich $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ alloy lattices matched to the GaP (001) substrate up to temperatures of $600°$C. Transformation of bonds, strain and coherency strain energies at the phase separation are taken into account. The alloys are considered to be strictly regular solutions. The strain energies of the alloys were calculated with the interaction parameters estimated by the valence force field model. It is shown that $GaAs_xN_yP_{1-x-y}$, having one mixed sublattice, are more promising from the spinodal decomposition standpoint than $In_xGa_{1-x}N_yP_{1-y}$, with two mixed sublattices.

Keywords: Quaternary alloys; spinodal decomposition.

Describimos las regiones de descomposición espinodal de las aleaciones $GaAs_xN_yP_{1-x-y}$ y $In_xGa_{1-x}N_yP_{1-y}$ crecidas sobre el substrato GaP (001) hasta una temperatura de $600°$C. Se tomó en cuenta la transformación de los enlaces, las energías de deformación y de deformación de coherencia en la separación de fase. Las aleaciones se consideran como soluciones estrictamente regulares. Las energías de deformación de las aleaciones se calculan con los parámetros de interacción estimados por el modelo de campo de fuerza de valencia. Se muestra que las aleaciones que tienen una subred de mezclado $GaAs_xN_yP_{1-x-y}$ son más prometedoras desde el punto de vista de la descomposición espinodal que las aleaciones con dos subredes de mezclado $In_xGa_{1-x}N_yP_{1-y}$.

Descriptores: Aleaciones cuaternarias; descomposición espinodal.

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1. Introduction

Low N-content III-V alloys have recently attracted considerable research attention. It has been found that incorporating low concentrations of N has a profound effect on the electronic properties of III-N-V alloy semiconductors composed of (B, Al, Ga, In), (N, P, As, Sb) [1,2]. A reduction of the band gap exceeding 0.1 eV per atomic percent of N content was observed in GaN_xAs_{1-x} for $x < 0.015$ [3]. Model calculations of the band structure of some of the group III-N-V alloys have shown that the reduction of the band gap is due to the highly localized nature of the perturbation introduced by N atoms [2,4-7]. Key devices for communications and information terminals are optoelectronic and microwave devices, typically lasers, light emitting diodes, heterojunction field-effect transistors and monolithic microwave integrated circuits. All these devices are fabricated by III-V alloy heterostructures [8]. The major interests are directed to quaternary alloys where a variation of the band gap can be reached without changing a lattice parameter. There are two types of quaternary III-V alloys that are the alloys having one and two mixed sublattices. The GaP-rich $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ alloys are considered. The large difference between the atomic sizes of nitrogen, phosphorus and arsenic gives rise to the significant strain energy of such alloys. The strain energy provides the tendency to phase separation that

can lead to the thermodynamically unstable states with respect to spinodal decomposition [9,10]. These unstable states may be produced as transformation of a homogeneous alloy into a two-phase system [11]. This decomposition leads to an occurrence of the coherency strain energy due to the stress between both formed regions with different compositions and these regions and the other part of an alloy [11]. The increase in internal energy due to the coherency strain energy decreases the spinodal decomposition range.

$GaAs_xN_yP_{1-x-y}$ belong to $A^{III}B_x^V C_y^V D_{1-x-y}^V$-type alloys where the anions (As, N and P) are surrounded by only one-type cations (Ga). Therefore, the decomposition of these alloys resulting in an exchange of lattice sites between the anions does not change the concentrations of the bonds. Accordingly, the spinodal decomposition range of $GaAs_xN_yP_{1-x-y}$ depends only on the strain and coherency strain energies. $In_xGa_{1-x}N_yP_{1-y}$ relate to the $A_x^{III}B_{1-x}^{III} C_y^V D_{1-y}^V$-type quaternary alloys. An exchange of lattice sites between cations or anions in such alloys leads to the transformation of the bonds described by the reaction $nA - D + nB - C \rightarrow nA - C + nB - C$ $(1 \leq n \leq 4)$ [12,13]. The transformation of the bonds should change the free energy of the alloy [12,13]. Thus, the spinodal decomposition range of $In_xGa_{1-x}N_yP_{1-y}$ depends on the strain and coherency strain energies and transformation of the bonds.

The crystal structures of both types of the III-group nitride alloys are very internally strained. The internal strains should result in the significant strain energy and, accordingly, a tendency to spinodal decomposition. It is of interest to find what type of these alloys is more stable from the spinodal decomposition standpoint. The regular solution model as a "conventional" model for the description of both types of these alloys will be used. The aim of this study is to estimate the spinodal decomposition ranges of GaAs$_x$N$_y$P$_{1-x-y}$ and In$_x$Ga$_{1-x}$N$_y$P$_{1-y}$ alloys grown on GaP (001) taking into account the transformations of the bonds, strain and coherency strain energies.

2. Model

According to Gibb's classic treatment of phase stability, spinodal decomposition begins from the changes that are large in extent but small in degree [14], and develops when a negligibly small phase separation fluctuation decreases the free energy of an alloy. The initial stage of spinodal decomposition is accompanied by transfers of atoms to the distances of the order of a lattice parameter. It was shown [15] that in crystals, spinodal decomposition forms layers in a plane where their elastic energy is minimal. Accordingly, the transfers of atoms produce a thin two-layer region with a negligibly small difference in composition. The compositions of the layers formed at the initial stage of the decomposition can be considered to be constant values due to their small thickness. As decomposition develops, transfers of atoms and thickness of the layers become larger, and the composition of the layers varies with their thickness. Afterwards, the difference in mean concentrations of the phases increases continuously [16]. The phase separation in cubic crystals in the vicinity of the spinodal decomposition ranges should occur in the $\{100\}$ planes, since the relation between the stiffness coefficients $2C_{44} - C_{11} + C_{12} > 0$ is fulfilled [15]. The stiffness coefficients of the alloys were estimated as average values of the constituent compounds. In such a case, the elastic energy due to the occurrence of these layers is minimal [15].

The phase separation leads to the changes in the value x, y or both of them in two phases occurring in the decomposed alloy. An alloy reaches the spinodal decomposition range when the variation in its free energy becomes equal to zero $\delta f = 0$ [17]. This condition is fulfilled if one of two expressions

$$\frac{\partial^2 f}{\partial x^2}, \quad \frac{\partial^2 f}{\partial x^2} \times \frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y} \right)^2 \qquad (1)$$

becomes equal to zero [16]. The Helmholtz free energy of the homogeneous alloys grown on crystalline substrates can be represented as a sum:

$$f = f^C + u^S + u^L - Ts, \qquad (2)$$

where f^C, u^S, u^L are the free energy of the constituent compounds, strain and lattice mismatch energies, respectively, s is

the configurational entropy, and T is the absolute temperature. The negligibly small lattice mismatch between the alloy and substrate is introduced in order to include the coherency strain energy in our consideration. Since GaAs$_x$N$_y$P$_{1-x-y}$ have a mixed sublattice, they contain three types of chemical bonds: GaAs, GaN and GaP. The crystal lattice of the In$_x$Ga$_{1-x}$N$_y$P$_{1-y}$ alloys consists of mixed cation and anion sublattices, since two kinds of the atoms fill each of them. Thus, these alloys have four types of bonds: InN, InP, GaN and GaP. The free energies of the constituent compounds of GaAs$_x$N$_y$P$_{1-x-y}$ and In$_x$Ga$_{1-x}$N$_y$P$_{1-y}$ are given, respectively, as

$$f^C = x\mu^0_{\text{GaAs}} + y\mu^0_{\text{GaN}} + (1 - x - y)\,\mu^0_{\text{GaP}}, \qquad (3)$$

$$f^C = xy\mu^0_{\text{InN}} + x\,(1 - y)\,\mu^0_{\text{InP}} + y\,(1 - x)\,\mu^0_{\text{GaN}}$$
$$+ (1 - x)\,(1 - y)\,\mu^0_{\text{GaP}}, \qquad (4)$$

where μ^0_{InN} is the chemical potential of InN in the standard state. The strain energies [13,18] of GaAs$_x$N$_y$P$_{1-x-y}$ and In$_x$Ga$_{1-x}$N$_y$P$_{1-y}$ are written, respectively, as

$$u^S = xy\alpha_{\text{GaAs-GaN}}$$
$$+ x\,(1 - x - y)\,\alpha_{\text{GaAs-GaP}}$$
$$+ y\,(1 - x - y)\,\alpha_{\text{GaN-GaP}}, \qquad (5)$$

$$u^S = x\,(1 - x)\,y\alpha_{\text{InN-GaN}}$$
$$+ xy\,(1 - y)\,\alpha_{\text{InN-InP}}$$
$$+ x\,(1 - x)\,(1 - y)\,\alpha_{\text{InP-GaP}}$$
$$+ y\,(1 - x)\,(1 - y)\,\alpha_{\text{GaN-GaP}}, \qquad (6)$$

where $\alpha_{\text{GaAs-GaN}}$, $\alpha_{\text{GaAs-GaP}}$ and $\alpha_{\text{GaN-GaP}}$ are the interaction parameters per 1 mol of the strictly regular solutions GaAs$_x$N$_{1-x}$, GaAs$_x$P$_{1-x}$ and GaN$_x$P$_{1-x}$ corresponding to the GaAs$_x$N$_y$P$_{1-x-y}$ alloy. Similarly, $\alpha_{\text{InN-GaN}}$, $\alpha_{\text{InN-InP}}$, $\alpha_{\text{InP-GaP}}$ and $\alpha_{\text{GaN-GaP}}$ in (6) are the interaction parameters per 1 mole of the In$_x$Ga$_{1-x}$N, InN$_x$P$_{1-x}$, In$_x$Ga$_{1-x}$P and GaN$_x$P$_{1-x}$ ternary strictly regular solutions. Thus, the strain energy is represented by the interaction parameters between the constituent compounds of the alloy. The interaction parameters were obtained from the strain energies of the corresponding ternary alloys estimated by the valence force field model. These energies were interpolated, for example, for GaAs$_x$N$_{1-x}$ as $\alpha_{\text{GaAs-GaN}}x(1 - x)$. The strain energies of the ternary alloys were estimated by the valence force field model as in Ref. 19. The valence force field model describes the strained state of the III-V semiconductors using two constants. One constant is the elastic constant of the bond length, or a bond stretching constant. Another constant is the elastic constant of the angle between the bonds, or a bond bending constant. The strain energy of a unit cell of a binary compound with the zinc blende structure according to the valence force field model is given as [20]
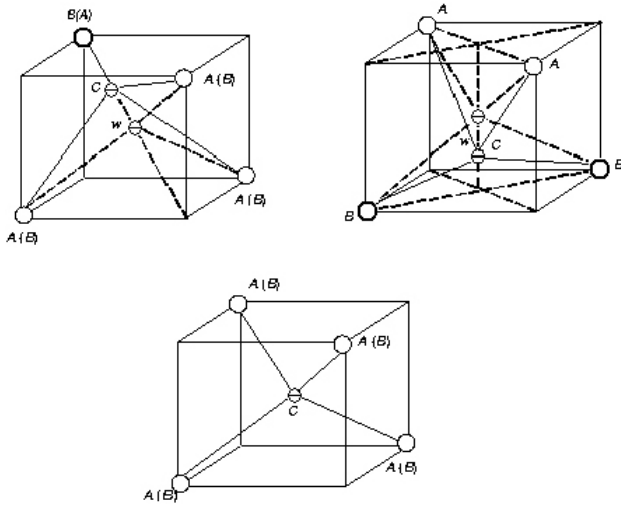
FIGURE 1. The 3A(B)1B(A)1C and 2A2B1C and 4A(B)1C tetrahedral cells.

$$u = \frac{1}{2}\alpha \left(\frac{3}{4R^2}\right) \sum_{i=1}^{4} \left[\Delta\left(r_i^1 \cdot r_i^1\right)\right]^2$$

$$+ \frac{1}{2}\sum_{s=1}^{2}\beta^s \left(\frac{3}{4R^2}\right) \sum_{i,j>i} \left[\Delta\left(r_i^s \cdot r_j^s\right)\right]^2,$$

where α and β are the bond-stretching and bond-bending elastic constants, respectively; R is the undistorted bond length; $\Delta\left(r_i^1 \cdot r_i^1\right) = R_i^2 - r_i^2$ and

$$\Delta\left(r_i^s \cdot r_j^s\right) = R^2 \cos\varphi_0 - r_i^s r_j^s \cos\varphi$$

are the scalar variations, where r_i^s and r_j^s are the bond vectors about atom s; $\varphi_0 = 109.47^0$ and φ are the angles between the bonds in the undistorted and distorted crystals, respectively. The strain energy of the ternary alloys was estimated as a sum of the deformation energies of the tetrahedral cells of the same size. The tetrahedral cells consist of four atoms from the mixed sublattice in the corners and one atom from another sublattice in the center, as shown in Fig. 1. The displacements of the central atoms were calculated by the minimum condition of the deformation energy of the cells.

The lattice mismatch energy of an epitaxial layer on a substrate with (001) orientation is given as [21]

$$u^L = \frac{(C_{11} - C_{12})(2C_{11} + C_{12})}{C_{11}} \left(\frac{a - a_S}{a_S}\right)^2,$$

where a and a_S are the lattice parameters of the alloy and substrate, respectively and C_{11}, C_{12} are the stiffness coefficients expressed as

$$C_{11} = xC_{11}^{GaAs} + yC_{11}^{GaN} + (1-x-y)C_{11}^{GaP}$$

$$C_{12} = xC_{12}^{GaAs} + yC_{12}^{GaN} + (1-x-y)C_{12}^{GaP}$$

and

$$C_{11} = xyC_{11}^{InN} + x(1-y)C_{11}^{InP} + x(1-y)C_{11}^{GaN}$$

$$+ (1-x)(1-y)C_{11}^{GaP}$$

$$C_{12} = xyC_{12}^{InN} + x(1-y)C_{12}^{InP} + x(1-y)C_{12}^{GaN}$$

$$+ (1-x)(1-y)C_{12}^{GaP}$$

for the $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$, respectively.

The configurational entropy of the alloys considered is obtained by the formula $s = k_B \ln g$, where g is the degeneracy factor.

The factor g for the $GaAs_xN_yP_{1-x-y}$ alloys is given as

$$g = \frac{(N_{As} + N_N + N_P)!}{N_{As}!N_N!N_P!},$$

and for the $In_xGa_{1-x}N_yP_{1-y}$ alloys as

$$g = \frac{(N_{In} + N_{Ga})!}{N_{In}!N_{Ga}!} \times \frac{(N_N + N_P)!}{N_N!N_P!},$$

where N_N, N_{Ga}, N_P, N_{In} and N_{As} are the numbers of atoms N, Ga, P, In and As, respectively.

Therefore, the configurational entropies of $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ are expressed, respectively, by the equations

$$s = -R\left[x\ln x + y\ln y + (1-x-y)\ln(1-x-y)\right], \quad (7)$$

$$s = -R[x\ln x + (1-x)\ln(1-x)$$

$$+ y\ln y + (1-y)\ln(1-y)]. \quad (8)$$

The conditions (1) for $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ considering (2-8) can be rewritten, respectively, as

$$-2\alpha_{GaAs-GaP} + \frac{RT(1-y)}{x(1-x-y)} + \frac{\partial^2 u^L}{\partial x^2} = 0, \quad (9)$$

$$\left[-2\alpha_{GaAs-GaP} + \frac{RT(1-y)}{x(1-x-y)} + \frac{\partial^2 u^L}{\partial x^2}\right]$$

$$\times \left[-2\alpha_{GaN-GaP} + RT\frac{RT(1-x)}{y(1-x-y)} + \frac{\partial^2 u^L}{\partial y^2}\right]$$

$$- \left(\alpha_{GaAs-GaN} - \alpha_{GaAs-GaP} - \alpha_{GaN-GaP}\right.$$

$$\left. - \frac{RT}{1-x-y} + \frac{\partial^2 u^L}{\partial x \partial y}\right)^2 = 0, \quad (10)$$

and

$$\alpha_{InN-GaN}y + \alpha_{InP-GaP}(1-y) - \frac{RT}{2x(1-x)}$$

$$+ \frac{\partial^2 u^L}{\partial x^2} = 0, \quad (11)$$

$$\left\{ 2\left[\alpha_{\text{InN–GaN}}y + \alpha_{\text{InP–GaP}}(1-y)\right] - \frac{RT}{x(1-x)} + \frac{\partial^2 u^L}{\partial x^2} \right\}$$

$$\times \left\{ 2\left[\alpha_{\text{InN–InP}}x + \alpha_{\text{GaN–GaP}}(1-x)\right] - \frac{RT}{y(1-y)} + \frac{\partial^2 u^L}{\partial y^2} \right\}$$

$$+ \left[\begin{array}{l} \mu_{\text{InN}}^0 + \mu_{\text{GaP}}^0 - \mu_{\text{InP}}^0 - \mu_{\text{GaN}}^0 + \left(\alpha_{\text{InN–GaN}} - \alpha_{\text{InP–GaP}}\right)(1-2x)+ \\ + \left(\alpha_{\text{InN–InP}} - \alpha_{\text{GaN–GaP}}\right) + \frac{\partial^2 u^L}{\partial x \partial y} \end{array} \right]^2 = 0. \qquad (12)$$

The term $\mu_{\text{InN}}^0 - \mu_{\text{InP}}^0 - \mu_{\text{GaN}}^0 + \mu_{\text{GaP}}^0$ in (12) contributes to the transformation of the bonds.

3. Results and Discussion

GaAs$_x$N$_y$P$_{1-x-y}$ and In$_x$Ga$_{1-x}$N$_y$P$_{1-y}$ alloys are grown by molecular beam epitaxy and metalorganic vapor-phase epitaxy with growth temperatures of 600°C or lower [22,23]. Therefore, the spinodal decomposition ranges were estimated at temperatures renging from 0 to 600°C. The value $\mu_{\text{InN}}^0 - \mu_{\text{InP}}^0 - \mu_{\text{GaN}}^0 + \mu_{\text{GaP}}^0$ was estimated as

$$\mu_{InN}^0 - \mu_{InP}^0 - \mu_{GaN}^0 + \mu_{GaP}^0 = \Delta h - T\Delta s$$

$$+ \int_{298.15}^{T} \Delta c\, dT - T \int_{298.15}^{T} \frac{\Delta c}{T}\, dT,$$

where $\Delta h = h_{InN} - h_{InP} - h_{GaN} + h_{GaP}$;

$$\Delta s = s_{InN} - s_{InP} - s_{GaN} + s_{GaP};$$

$$\Delta c = c_{InN}^P - c_{InP}^P - c_{GaN}^P + c_{GaP}^P;$$

and h_{InN}, s_{InN} and c_{InN}^P are the enthalpy, the entropy at the standard state and the specific heat capacity at constant pressure of InN, respectively. This term takes into acount the transformation of the bonds in Eq. (12). The thermodynamic, elastic and structural characteristics of the constituent compounds were taken from [24]. The interaction parameters

$$\alpha_{GaN-GaP} = 155.9\text{kJ/mole},$$

$$\alpha_{GaAs-GaP} = 5.786\text{kJ/mole},$$

$$\alpha_{GaN-GaAs} = 215.2\text{kJ/mole},$$

$$\alpha_{InN-InP} = 96.16\text{kJ/mole},$$

$$\alpha_{InN-GaN} = 45.32\text{kJ/mole}$$

and $\qquad \alpha_{InP-GaP} = 25.11\text{kJ/mole}$

were estimated from the strain energy of the corresponding ternary alloys by the approach from Ref. 25. The bond stretching and bond bending elastic constants of GaAs, GaN, GaP, InN and InP were taken from [20,26]. The other interaction parameters used in the calculations were taken from [26]. The lattice parameters of $GaAs_xN_yP_{1-x-y}$ are given as

$a = xa_{GaAs} + ya_{GaN} + (1-x-y)a_{GaP}$ and for $In_xGa_{1-x}N_yP_{1-y}$ as

$$a = xya_{InN} + x(1-y)a_{InP} + y(1-x)a_{GaN}$$
$$+ (1-x)(1-y)a_{GaP}.$$

In the estimates, we supposed that the lattice parameters of the alloys and the substrate are close to each other ($a \approx a_{GaP}$). Then, the concentrations of As and In in the $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ alloy lattice considered, matched to GaP, are given, as

$$x = \frac{a_{GaP} - a_{GaN}}{a_{GaAs} - a_{GaP}}y$$

and

$$x = \frac{y(a_{GaP} - a_{GaN})}{a_{InP} - a_{GaP} + y(a_{InP} - a_{InN} + a_{GaN} - a_{GaP})},$$

respectively. Accordingly, the spinodal decomposition ranges of these alloys are functions of one independent variable, which is the nitrogen concentration. The spinodal decomposition ranges of the GaP-rich alloys are demonstrated in Fig. 2.

The GaP-rich $GaAs_xN_yP_{1-x-y}$ alloys are successfully grown by molecular beam epitaxy. As can be seen from Fig. 2, $GaAs_{0.87}N_{0.07}P_{0.06}$ and $GaAs_{0.66}N_{0.03}P_{0.31}$ alloys [27,22] are inside and outside, respectively, the spinodal decomposition range at the growth temperature. At the same time, the lattice mismatched $In_{0.15}Ga_{0.85}N_{0.01}P_{0.99}$ ($a = 5.504$Å) and $In_{0.1}Ga_{0.9}N_{0.015}P_{0.985}$ ($a = 5.478$Å) grown by metalorganic vapor phase epitaxy [24] are outside but near the boundary of the spinodal decomposition range at their growth temperatures. However, as can be seen from Fig. 2, the spinodal decomposition range of $In_xGa_{1-x}N_yP_{1-y}$ is much more extensive than that of $GaAs_xN_yP_{1-x-y}$. Accordingly, $GaAs_xN_yP_{1-x-y}$ are more promising than $In_xGa_{1-x}N_yP_{1-y}$ from the spinodal decomposition standpoint. The bond transformation occurring during the phase separation of $In_xGa_{1-x}N_yP_{1-y}$ leads to a dramatic increase in the spinodal decomposition range. The transformation of In-P and Ga-N bonds into In-N and Ga-P ones is thermodynamically profitable, since the sum of the free energies of InN and GaP is significantly smaller that
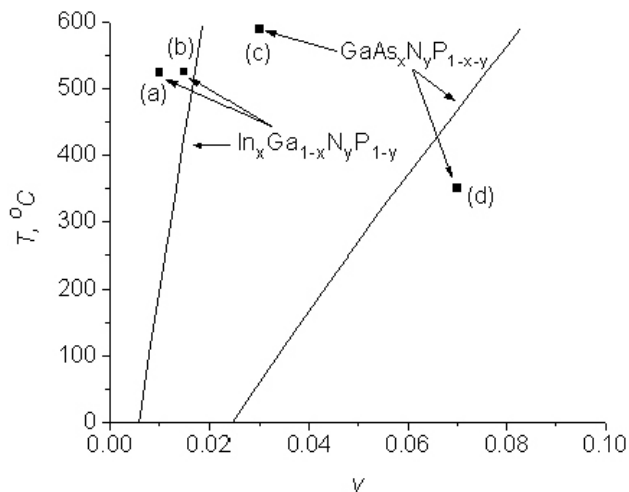
FIGURE 2. Spinodal decomposition ranges of the GaP-rich $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ alloys. The experimental values (a) $x = 0.15, y = 0.01$ and (b) $x = 0.1, y = 0.015$ correspond to $In_{0.15}Ga_{0.85}N_{0.01}P_{0.99}$ and $In_{0.1}Ga_{0.9}N_{0.015}P_{0.985}$ alloys, respectively, (c) $x = 0.66, y = 0.03$ and (d) $x = 0.87$, $y = 0.07$ are the experimental values of $GaAs_{0.66}N_{0.03}P_{0.31}$ and $GaAs_{0.87}N_{0.07}P_{0.06}$ alloys, respectively.

that of InP and GaN. The lengths of In-N and Ga-P bonds are smaller than those of In-P and Ga-N ones. Therefore, the bond transformation reaction during spinodal decomposition is given as $nIn-P+nGa-N \rightarrow nIn-N+nGa-P$. In line with this reaction, one of two thin layers produced becomes

GaP-rich and another layer becomes InN-rich in comparison with the homogeneous alloy. Therefore, in spite of the significant strain energy, the $GaAs_xN_yP_{1-x-y}$ alloys in the large composition regions are outside the spinodal decomposition range at the growth and lower temperatures.

Nevertheless, it is known that these alloys are very difficult to grow in certain compositional regions [28]. One of the experimental observations in nitride-based alloys is that there are serious compositional inhomogeneity problems for both group III-nitride alloys and GaN-based mixed anion nitride alloys such as $In_xGa_{1-x}N$ and $GaAs_xN_{1-x}$[29-32]. These difficulties are observed in all growth techniques used for these semiconductors. The compositional immiscibility problem appears in association with an unstable two-phase region in the composition plane [33]. The same situation also can be expected for both group-III-nitride quaternary alloys.

4. Conclusions

In summary, we have described spinodal decomposition ranges of $GaAs_xN_yP_{1-x-y}$ and $In_xGa_{1-x}N_yP_{1-y}$ lattice-matched to GaP, considering the transformations of the bonds, strain and coherency strain energies. The strain energy is estimated by the valence force field model with the bond stretching and bond bending elastic constants of GaP. From the spinodal decomposition standpoint, $GaAs_xN_yP_{1-x-y}$ alloys are more promising than $In_xGa_{1-x}N_yP_{1-y}$ones.

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